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For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: CRYSTALLIZING MURG PROTEIN, METHODS OF MAKING AND USING MODELS THEREOF FOR INHIBITION AND STIMULATION VIA COMPOUNDS

(57) Abstract: The present invention relates to crystals of the Escherichia coli MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional sturctures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three dimensional coordinates described herein. The present invention relates to methods of crystallizing MurG proteins. The present invention relates to models of three dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three dimensional structure dimensional structure of crystals of the Escherichia coli MurG. The present invention also relates to models of the three dimensional structures of the α-carbon backbone and the α-carbon backbone and conserved amino acid residue sidechains of UDP-glycosyltransferases and MurG proteins and of the binding sites thereof. The present invention also relates to methods of drug design using models of this invention, the compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins, and compositions comprising compounds identified using the models of this invention for therapeutic or diagnositic uses. Also, the present invention relates to methods of making models of the present invention.

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INTERNATIONAL SEARCH REPORT

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A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) :C12N 9/00
US CL :435/183

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 435/183

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

STN: West

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 99/38958 A1 (PRINCETON UNIVERSITY) 05 August 1999, see entire document.	1-2
X	US 5,068,191 A (CLAUSEN et al.) 26 November 1991, see entire document.	45-51

☐ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

*	Special categories of cited documents:	"T"	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"A"	document defining the general state of the art which is not considered to be of particular relevance	"X"	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"E"	earlier document published on or after the international filing date	"Y"	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"L"	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"&"	document member of the same patent family
"O"	document referring to an oral disclosure, use, exhibition or other means		
"P"	document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search 24 JANUARY 2002	Date of mailing of the international search report 13 FEB 2002
Name and mailing address of the ISA/US Commissioner of Patents and Trademarks Box PCT Washington, D.C. 20231 Facsimile No. (703) 305-3230	Authorized officer AMY HARTTER Telephone No. (703) 308-0196

Form PCT/ISA/210 (second sheet) (July 1998)*

INTERNATIONAL SEARCH REPORT

International application No.
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Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☐ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

Please See Extra Sheet.

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. ☒ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
1-2; 45-51

4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐ The additional search fees were accompanied by the applicant's protest.

☐ No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US01/11500

BOX II. OBSERVATIONS WHERE UNITY OF INVENTION WAS LACKING
This ISA found multiple inventions as follows:

Group I, Claims 1-2, drawn to the crystalline form of the MurG protein
Group II, Claims 3-6, drawn to the 3-D structure of the crystalline form of the MurG protein.
Group III, Claims 7-8, drawn to the 3-D structure of the donor nucleotide binding site of the MurG protein.
Group IV, Claim 9, drawn to the 3-D structure of the acceptor binding site of the MurG protein.
Group V, Claim 10, drawn to the 3-D structure of the membrane association site of the MurG protein.
Group VI, Claims 11-19, drawn to the computer image of the 3-D MurG protein.
Group VII, Claims 20-23, drawn to the 3-D image of the 3-D image of an alpha-carbon backbone.
Group VIII, Claims 24-28, drawn to the 3-D computer image of the 3-D structure of a donor nucleotide of a donor nucleotide binding site of the MurG protein.
Group IX, Claims 29-33, drawn to the 3-D computer image of a 3-D structure of an acceptor binding site of the MurG protein.
Group X, Claims 34-38, drawn to the 3-D computer image of the 3-D structure of a membrane association site of the MurG protein.
Group XI, Claims, 39-41, drawn to the computer readable medium encoded with a set of 3-D coordinates of a MurG protein.
Group XII, Claim 42, drawn to the computer readable medium encoded with a set of 3-D coordinates of a donor nucleotide binding site of a MurG protein.
Group XIII, Claim 43, drawn to the computer readable medium with a set of 3-D coordinates of an acceptor binding site of the MurG protein.
Group XIV, Claim 44, drawn to a computer readable medium encoded with 3-D coordinates of a membrane association site of the MurG protein.
Group XV, Claims 45-51, drawn to a method for identifying a potential inhibitor of a UDP-glycotransferase enzyme.
Group XVI, Claims 52-87, drawn to a model of UDP-glycotransferase where the model represents a 3-D structure.
Group XVII, Claims 88-97, drawn to a model a donor nucleotide binding site of a UDP-glycosyltransferase protein.
Group XVIII, Claims 98-107, drawn to a model of an acceptor binding site of a UDP-glycotransferase protein.
Group XIX, Claims 108-116, drawn to a model of a membrane association site of a UDP-glycotransferase protein.
Group XX, Claims 117-132, drawn to a computer-assisted method of structure based drug design of bioreative compounds,
Group XXI, Claims 133-134, drawn to a model of a 3-D structure of a MurG protein.
Group XXII, Claims 135-141, drawn to a composition for inhibiting the activity of a glycotransferase.
Group XXIII, Claim 142, drawn to a composition for stimulating the activity of glycotransferase.
Group XXIV, Claims 143-148, drawn to a method to determine the 3-D structure of a MurG protein.

This International Searching Authority considers the international application does not comply with the requirements of unity of invention (Rules 13.1, 13.2 and 13.3) for the reasons indicated below: The inventions listed in Groups 1-24 do not relate a single inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: the special technical feature for Group I is that the MurG is being claimed in its crystalline form. In Group II the special technical feature is that the 3-D structure of the crystalline form of the MurG protein is being claimed. Group III's special technical feature is that the Group is claiming the 3-D structure of the binding site of MurG. In Group IV the special technical feature emerges as the 3-D structure of the acceptor binding site of the MurG protein. Group V embraces the special technical feature of the 3-D structure of a membrane association site. In Group VI the special technical feature is that of the 3-D computer image of the 3-D structure of the MurG protein. Group VII has the special technical feature of a 3-D structure of a 3-D structure of an alpha-carbon backbone of the MurG protein. Group VIII deals with the special technical feature of the 3-D computer image of the 3-D structure of a donor nucleotide binding site of the instant protein. Group IX involves the special technical feature of the 3-D computer image of the 3-D structure of an acceptor binding site. Group X develops the special technical feature of the 3-D computer image of the 3-D structure of a membrane association site of the MurG protein. In Group XI the subject of the special technical feature of a computer readable medium encoded within a set of 3-D coordinates of the MurG protein are described. Group XII addresses the technical feature of a computer readable medium that is encoded with a set of 3-D coordinates of a donor nucleotide binding site of the MurG protein. In Group XIII is drawn to the special technical feature of a computer readable medium with a 3-D set of coordiantes to accommodate the acceptor binding site of a MurG protein. Group IV involves the special technical feature of a computer readable medium that is encoded with a set of 3-D coordinates that is used for the membrane association site of the MurG protein. Group V is involved with the special technical feature of a method for identifying a potential inhibitor a UDP-glycotransferase enzyme. The special technical feature of Group XVI is that of a 3-D model of UDP-glycotransferase. Group XVII addresses the special technical feature of a model of a donor nucleotide binding site of UDP-glycotransferase. Group XVIII addresses the special technical feature of the model of an acceptor binding site of a UDP glycotransferase. Group XIX consists of the special technical feature of a model of the membrane association site of a UDP-glycotransferase. In Group XX we see that the special

technical feature is that of a computer-assisted method of structure based drug design. In Group XXI the special technical feature that emerges is that of a model of a 3-D structure of a MurG protein. Group XXII deals with the special technical feature of a composition for inhibiting the activity of a glycotransferase. Group XXIII addresses the special technical feature of a composition for the stimulation of activity of a glycotransferase. Finally Group XXIV speaks to the special technical feature of a method to determine the 3-D structure of the MurG protein.

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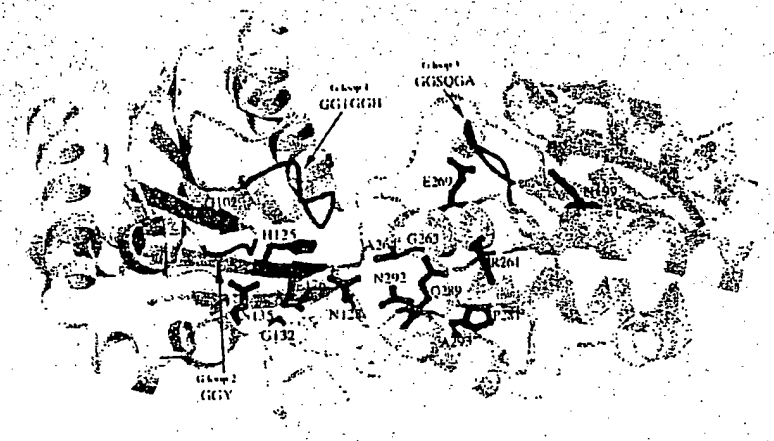
— *without international search report and to be republished upon receipt of that report*

[Continued on next page]

(54) Title: METHODS OF MAKING MODELS, METHODS OF USING MODELS OF MURG, COMPOUNDS THAT BIND, INHIBIT OR STIMULATE MURET PROTEINS, AND THERAPEUTIC COMPOSITIONS THEREOF



(57) Abstract: The present invention relates to crystals of the *Escherichia coli* MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional sturctures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three dimensional coordinates described herein. The present invention relates to methods of crystallizing MurG proteins. The present invention relates to models of three dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three dimensional structure dimensional structure of crystals of the *Escherichia coli* MurG. The present invention also relates to models of the three dimensional structures of the α-carbon backbone and the α-carbon backbone and conserved amino acid residue sidechains of UDP-glycosyltransferases and MurG proteins and of the binding sites thereof. The present invention also relates to methods of drug design using models of this invention, the compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins, and compositions comprising compounds identified using the models of this invention for therapeutic or diagnositic uses. Also, the present invention relates to methods of making models of the present invention.

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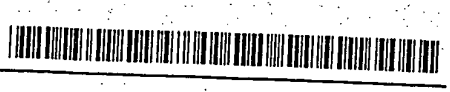

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

METHODS OF MAKING MODELS, METHODS OF USING MODELS OF MURG, COMPOUNDS THAT BIND, INHIBIT OR STIMULATE MURG PROTEINS, AND THERAPEUTIC COMPOSITIONS THEREOF

FIELD OF THE INVENTION

The present invention relates to crystals of the *Escherichia coli* MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone of the MurG protein and images thereof. The present invention further relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional structures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and the conserved amino acid residue sidechains of the MurG protein, the donor nucleotide binding site, the acceptor binding site, and the membrane association site. The present invention relates to methods of crystallizing MurG proteins.

The present invention relates to models of three dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three dimensional structure of crystals of the *Escherichia coli* MurG. The present invention also relates to models of the three dimensional structures of the α-carbon backbone of UDP-glycosyltransferases and MurG proteins. The present invention further relates to models of the three dimensional structure of the α-carbon backbone and conserved amino acid residue sidechains of gUDP-glycosyltransferases, in particular, MurG proteins. The present invention further relates to models of the three-dimensional structures of donor nucleotide binding sites, acceptor binding sites, and membrane association sites of UDP-glycosyltransferases, in particular, MurG proteins. The present invention also relates to methods of drug design using models of this invention. The present invention further relates to compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins. The present invention relates to compositions comprising compounds identified using the models of this invention for therapeutic or diagnositic uses. Also, the present invention relates to methods of making models of the present invention.

BACKGROUND OF THE INVENTION

The increasing frequency of resistance to existing antibiotics represents a serious public health threat. Structural and mechanistic information on essential bacterial enzymes could lead to the development of antibiotics that are active against resistant microorganisms. Both gram positive and gram negative bacterial cells are surrounded by a cross-linked carbohydrate polymer, peptidoglycan, which protects them from rupturing under high osmotic pressures. Many of the best antibiotics function by inhibiting peptidoglycan synthesis, which ultimately causes cell lysis. In recent years, intense effort has been focused on determining the structures of the enzymes that synthesize peptidoglycan. Structures of several of the early enzymes in the biosynthetic pathway have been reported (Benson *et al.*, 1995; Bertrand *et al.*, 1997; Fan *et al.*, 1994; Skarzynski *et al.*, 1996); however, the later enzymes have proven more difficult to study because both they and their substrates are membrane-associated.

MurG is the last enzyme involved in the intracellular phase of peptidoglycan synthesis (Bugg & Walsh, 1993). It catalyzes the transfer of N-acetyl glucosamine

(NAG) from UDP to the C4 hydroxyl of a lipid-linked N-acetylmuramoyl pentapeptide (NAM) to form a ?-linked NAG-NAM disaccharide that is transported across the cell membrane where it is polymerized and cross-linked (Fig. 1). In bacterial cells MurG associates with the cytoplasmic surface of the membrane (Bupp & van Heijenoort, 1993). However, we have found that *E. coli* MurG can be solubilized at high concentrations in active form (Ha *et al.*, 1999).

The elucidation of the protein structure of a MurG protein is of importance in the identification and formulation of anti-bacterial agents. Until the discovery of the present invention, the structure and resulting mechanism by which MurG functions was not known. Thus, despite the important role of MurG in peptidoglycan synthesis, development of useful agents for treatment or diagnosis of disease was hindered by lack of structural information of the protein.

In order to obtain structural information on a MurG protein, it is important to have purified, active enzyme. The demonstration of activity requires a suitable assay, which in turn requires access to the natural substrates or analogues thereof. The study of MurG was hampered by difficulties obtaining and handling the lipid-linked NAM substrate (commonly known as Lipid I). This problem was overcome by Walker and coworkers, who developed a synthetic route to a set of substrate analogues of Lipid I that were shown to function as glycosyl acceptors in a glycosyl transfer reaction catalyzed by MurG. Some of these substrate analogues are freely water soluble, making it possible to monitor the activity of purified *E. coli* MurG in buffer in the absence of natural or artificial membranes or detergents.

The linear nucleic acid and amino acid sequences of *E. coli* MurG were reported in 1992. Subsequently, the nucleic acid and amino acid sequence of *B. subtilus* MurG was reported. Since then, many bacterial genomes have been sequenced and the information has been deposited in databases. Information based only on linear sequences, however, cannot accurately predict the three-dimensional structure of the protein and its functional domains.

Therefore, there is a need in the art to elucidate the three-dimensional structure of a MurG protein. One three dimensional structure of a MurG protein can be used to construct models of other MurG proteins and to facilitate the structure determination of crystalline forms of other MurG proteins. Structures and models of MurG proteins can

also be used to design proteins containing only the donor binding site or the acceptor binding site. These proteins can be used in assays, including NMR-based assays, to identify -- or characterize the mode of binding of -- ligands that bind in or near the vicinity of the substrates. These ligands or compounds can then be used as leads for the design of inhibitors that have therapeutic activity. Structures and models of MurG proteins can also be used in computer-based drug design.

SUMMARY OF THE INVENTION

The present invention relates to crystalline *Escherichia coli* MurG protein. Obtaining such crystals is an unexpected result. It is well known in the protein crystallographic art that obtaining crystals of quality sufficient for determining the structure of a protein is unpredictable. In particular, obtaining crystals of quality sufficient for determining the three-dimensional (3-D) structure of MurG has not been achievable until the crystallization of MurG as disclosed in the present application. As such, determination of the three-dimensional structure of MurG has not been possible until the discovery of the present invention. Additionally, until the discovery of the present invention, derivation of the three-dimensional structure and models of other MurG proteins has not been possible. The present inventors are also the first to define the three-dimensional structure and provide three-dimensional models for drug design for MurG proteins.

Accordingly, one object of the present invention is to provide crystals of sufficient quality to obtain a determination of the three-dimensional atomic coordinates and structures of MurG to high resolution, preferably to the resolution of less than 2.0 angstroms (Å). The present invention also provides methods for producing crystalline MurG protein.

The value of the crystals of *E. coli* MurG protein extends beyond merely being able to obtain such crystals. The knowledge obtained concerning the MurG crystal structure, for example, has been used by the present inventors to define the heretofore unknown tertiary structure of the MurG protein and to identify the location of the glycosyl donor and glycosyl acceptor binding domains, as well as the location of the amino acid residues that are invariant in all MurG proteins. This information can be used to design inhibitors of MurG that have therapeutic utility. The atomic coordinates of *E.*

coli MurG also are used to model the heretofore unknown tertiary structures of other MurG proteins having substantially related linear amino acid sequences, such as for MurG proteins from other microorganisms. It is anticipated that homology models can be constructed even from amino acid sequences with relatively low homology because the present inventors have identified the location of the invariant amino acid residues in MurG. The relative spatial orientations of such residues is expected to be conserved in all MurG proteins.

Comparison of nucleic acid and amino acid sequences of MurG proteins indicates that the linear amino acid sequences can vary significantly. Homology between MurG proteins from different microorganisms varies from less than 30% to greater than 90%, reflecting the evolutionary relationship between the organisms. The low homology between distantly related MurG homologues is not believed to reflect significantly different folded structures. It is well known that many amino acid sequences are capable of adopting the same general fold. *E. coli* MurG contains an alpha/beta folding pattern, one of the most common folds known in proteins. It is likely that all MurG homologues contain a similar alpha/beta fold despite the differences in the linear amino acid sequences. What gives these proteins their identity is not the general fold, but the specific details – *i.e.*, the presentation of certain amino acids on the folded structure. The present inventors have identified the location in *E. coli* MurG of a set of residues that are invariant in all MurG homologues. It is to be expected that these residues would adopt a similar spatial location with respect to the folded structure in all MurG homologues. Therefore, these invariant residues, which have been selected by evolution as the critical residues for the binding and catalytic function of the protein, provide essential information on the location of the active site and on critical contacts to the substrates/products. They also serve as constraints that make it possible to predict the three-dimensional structures even of distantly related MurG homologues. Thus, knowledge of the three-dimensional structure of the *E. coli* MurG protein has provided a starting point for investigation into the structure of all MurG proteins.

Accordingly, a object of the present invention is to provide information regarding the atomic coordinates and three-dimensional structures of (1) the MurG protein, (2) the α-carbon backbone of the MurG protein, (3) the α-carbon backbone and conserved

amino acid residues of the MurG protein, (4) the donor nucleotide binding site, (5) the acceptor binding site, and (6) the membrane association site MurG proteins.

It is also an object of this invention to solve the three-dimensional structure of UDP-glycosyltransferases, in particular target MURG proteins, and to determine their structure and/or atomic coordinates. Further, it is an object of this invention to use the structure or atomic coordinates of the *E. coli* MurG crystal to solve the structure of different MURG protein crystals, or a crystal of a mutant protein, homolog or co-complex of MurG.

The present invention relates to models of three dimensional structures of UDP-glycosyltransferases, in particular MurG proteins, based on the atomic coordinates of crystalline *E. coli* MurG protein.

It is a further object of this invention to provide UDP-glycosyltransferase enzyme mutants characterized by one or more different properties as compared with wild-type MURG. These properties include altered surface charge, increased stability to subunit dissociation, altered substrate specificity or higher specific activity. MURG mutants are useful to identify those amino acids that are most important for the enzymatic activity of MURG. This information, in turn, allows the design of improved inhibitors of MURG as compared with peptidic MURG inhibitors.

Another object of the present invention is to provide computer readable mediums encoded with a set of three-dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

Another embodiment of the present invention provides three-dimensional and two-dimensional computer images of the three dimensional structure of MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

The knowledge of the three dimensional structure of MurG also provides a means for designing proteins that have altered beneficial functions by analyzing the structure and interactions between individual amino acids of the protein. For example, the present inventors have shown that E. coli MurG consists of two domains separated by a cleft.

Noncovalent interactions between the two domains are not extensive. The present inventors have shown that the domains fold independently and can, therefore, be expressed independently either alone or as part of a recombinant protein containing the acceptor binding site from one MurG homologue and the donor binding site from another MurG homologue. It would be expected that the domains of other MurG proteins could also be expressed independently, either alone or as chimaeras with other MurG domains. Independently expressed domains of the protein are useful for discovering ligands that bind to the individual domains.

The knowledge of the three-dimensional structure of *E. coli* MurG protein and models of other MurG proteins also provides a means for designing and producing compounds that regulate, inhibit or antagonize functions of the MurG protein (i.e., structure based drug design). For example, chemical compounds can be designed to block binding of UDP-GlcNAc to a MurG protein using various computer programs and models.

It is also an object of this invention to use the structure coordinates and atomic details of MURG, or its mutants or homologues or co-complexes, to design, evaluate computationally, synthesize and use inhibitors of MURG that avoid the undesirable physical and pharmacologic properties of peptidic MURG inhibitors.

Another embodiment of the present invention is a composition comprising MurG protein in a crystalline form.

Yet another embodiment of the present invention is a method for producing crystals of MurG, comprising combining MurG protein in a suitable buffer with a suitable amount of a reservoir buffer containing a detergent, and inducing crystal formation to produce said MurG crystals.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1. Pathway for peptidoglycan biosynthesis.

Fig. 2. Overall architecture of MurG. **A.** Stereo view of the MurG structure. The N domain is shown in purple; the C domain is shown in green. The figure was generated with the programs MOLSCRIPT (Klaulis, 1991) and RASTER3D (Merrit & Murphy, 1994). **B.** Topology diagram of MurG.

Fig. 3. Identification of critical residues in MurG and related glycosyltransferases. **A.** Sequence alignment of *E. coli* MurG with homologs from seven other bacterial strains, deliberately chosen to represent a disparate group of organisms. The secondary structure of *E. coli* MurG is shown above the sequences. Gaps mapping to the loop regions of *E. coli* MurG suggest that some sequences include other structural elements. Residues highlighted in blue are invariant among the eighteen MurG sequences available. Residues highlighted in yellow are identical in 85% of the eighteen homologs, while in the remaining 15%, only closely related amino acid substitutions are found. Highly conserved residues that do not meet the stringent criteria established for highlighting are shown in the consensus sequence. A consensus motif for UDP-glucuronosyltransferases is also shown. Numbering is with respect to the overexpressed *E. coli* MurG construct, which contains an additional N-terminal methionine. **B.** Mapping of the G loops and other highlighted residues from Fig. 3a in red on the MurG structure. Side chains for highly conserved residues are also shown. **C.** Model for the proposed UDP-binding subdomain found in many UDP-glycosyltransferases based on the *E. coli* MurG structure. Conserved residues in UDP-glucuronosyltransferases are highlighted in red. Side chains are shown for residues that are located near the cleft and may be involved in substrate binding. The glutamate residue is proposed to interact with the ribose sugar. The dotted loop varies in length within the MurG family and in other UDP-sugar transferases, but the N and Q on the following helix are invariant. Note that the UDP-glucuronosyltransferases contain a conserved D preceding the Q, which is not shown on this model.

Fig 4. Structural analysis of the substrate binding pockets in MurG. **A.** Structural comparison between the C-terminal domain of phage T4 ?-glucosyltransferase (left) and the C-terminal domain of *E. coli* MurG (right). The aligned six ?-strands are magenta, the aligned ?-helices are orange, and the other structural elements are blue. In ?-glucosyltransferase, key residues involved in UDP binding are highlighted in yellow. The analogous residues in MurG are also highlighted in yellow. **B.** A close-up view of the proposed donor binding pocket in the MurG C domain with the docked UDP-GlcNAc. Conserved residues in MurG are colored magenta. The carbonyl oxygen of

residue I245 is shown in red, and its backbone nitrogen is shown in blue. C. The surface of *E. coli* MurG. The G loops and other conserved residues in MurG are colored magenta. The proposed membrane binding interface is also highlighted with hydrophobic residues in yellow and positively charged residues in blue.

DEFINITIONS

It is to be noted that the term "a" or "an" entity refers to one or more of that entity; for example, a compound refers to one or more compounds or at least one compound. As such, the terms "a" (or "an"), "one or more", and "at least one" can be used interchangeably herein.

It is also to be noted that the terms "comprising", "including" and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures (i.e., combinations) of two or more of the compounds.

According to the present invention, an isolated, or pure, protein, is a protein that has been removed form its natural milieu. As such, "isolated" and "biologically pure" do not necessarily reflect the extent to which the protein has been purified, An isolated protein of the present invention can be obtained from its natural source, can be produced using recombinant DNA technology or can be produced by chemical synthesis.

It is also to be noted that the terms "tertiary" and "three dimensional" can be used interchangeably.

It is also to be noted that reference to a "MurG protein" can also be recited as "MurG" and such terms can be used to refer to the complete MurG protein, a portion of the MurG protein, such as a polypeptide.

The following terms are also used herein:

The term "naturally occurring amino acids" means the L-isomers of the naturally occurring amino acids. The naturally occurring amino acids are glycine, alanine, valine, leucine, isoleucine, serine, methionine, threonine, phenylalanine, tyrosine, tryptophan, cysteine, proline, histidine, aspartic acid, asparagine, glutamic acid, glutamine, .gamma.-carboxyglutamic acid, arginine, ornithine and lysine. Unless specifically indicated, all amino acids referred to in this application are in the L-form.

The term "unnatural amino acids" means amino acids that are not naturally found in proteins. Examples of unnatural amino acids used herein, include racemic mixtures of selenocysteine and selenomethionine. In addition, unnatural amino acids include the D or L forms of nor-leucine, para-nitrophenylalanine, homophenylalanine, para-fluorophenylalanine, 3-amino-p2-benzylpropionic acid, homoarginine, and D-phenylalanine.

The term "positively charged amino acid" includes any naturally occurring or unnatural amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine.

The term "negatively charged amino acid" includes any naturally occurring or unnatural amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid.

The term "hydrophobic amino acid" means any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of naturally occurring hydrophobic amino acids are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine.

The term "hydrophilic amino acid" means any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples of naturally occurring hydrophilic amino acids are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

The term "MurG" refers to a UDP-glycosyltransferase that has a two domain strucuture, where each domain contains a set of invariant residues as shown in Figure 3a, including any mutant, homologue or co-complex or any similar enzyme that catalyzes the transfer of N-acetylglucosamine (GlcNAc) from UDP to the C4 hydroxyl of the lipid-linked MurNAc pentapeptide.

The term "mutant" refers to a MurG polypeptide, *i.e.*, a polypeptide displaying the biological activity of a wild-type MurG, characterized by the replacement of at least one amino acid from the wild-type, *E. coli* MURG sequence according to Ikeda, et al., Nucleic Acids Res. 1990, and Mengin-LeCreuix et al., Nucleic Acids Res. 1990. Such a

mutant may be prepared, for example, by expression of MURG cDNA previously altered in its coding sequence by PCR-based mutagenesis method.

MurG mutants may also be generated by site-specific incorporation of unnatural amino acids into MURG proteins using the general biosynthetic method of Noren, C. J., et al., Science, 244, pp. 182-188 (1989). In this method, the codon encoding the amino acid of interest in wild-type MURG is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis (described in detail, infra). A suppressor tRNA directed against this codon is then chemically aminoacylated in vitro with the desired unnatural amino acid. The aminoacylated tRNA is then added to an in vitro translation system to yield a mutant MURG enzyme with the site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant MURG by expression of MURG-encoding cDNAs in auxotrophic E. coli strains. Hendrickson, W. A. et al., EMBO J., 9(5), pp. 1665-1672 (1990). In this method, the wild-type or mutagenized MURG CDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "altered surface charge" means a change in one or more of the charge units of a mutant polypeptide, at physiological pH, as compared to wild-type MURG. This is preferably achieved by mutation of at least one amino acid of wild-type MURG to an amino acid comprising a side chain with a different charge at physiological pH than the original wild-type side chain.

The change in surface charge is determined by measuring the isoelectric point (pI) of the polypeptide molecule containing the substituted amino acid and comparing it to the isoelectric point of the wild-type MURG molecule.

The term "altered substrate specificity" refers to a change in the ability of a mutant MURG to cleave a substrate as compared to wild-type MURG.

The "kinetic form" of MURG refers to the condition of the enzyme in its free or unbound form or bound to a chemical entity at either its active site or accessory binding site.

A "competitive" inhibitor is one that inhibits MURG activity by binding to the same kinetic form, of MURG, as its substrate binds—thus directly competing with the

substrate for the active site of MURG. Competitive inhibition can be reversed completely by increasing the substrate concentration.

An "uncompetitive" inhibitor is one that inhibits MURG by binding to a different kinetic form of the enzyme than does the substrate. Such inhibitors bind to MURG already bound with the substrate and not to the free enzyme. Uncompetitive inhibition cannot be reversed completely by increasing the substrate concentration.

A "non-competitive" inhibitor is one that can bind to either the free or substrate bound form of MURG.

Those of skill in the art may identify inhibitors as competitive, uncompetitive or non-competitive, by computer fitting enzyme kinetic data using standard equations according to Segel, I. H., Enzyme Kinetics, J. Wiley & Sons, (1975). It should also be understood that uncompetitive or non-competitive inhibitors according to this invention may bind to the accessory binding site.

The term "homolog" means a protein having at least 25% amino acid sequence identity with MURG or any functional part of MURG, and including certain invariant amino acid residues corresponding to G14, G15, G18, H19, G104, H124, E125, G190, G191, S192, G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E.coli* MurG sequence set forth in Figure 3a) and also including three glycine rich loops. A homolog may contain some or all of the invariant residues.

The term "co-complex" means MURG or a mutant or homologue of MURG in covalent or non-covalent association with a chemical entity or compound.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a MurG molecule or portions thereof. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be covalent.

The term ".beta.-sheet" refers to the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

The terms "atomic coordinates" or "structure coordinates" refer to mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a

MurG molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

The term "heavy atom derivatization" refers to the method of producing a chemically modified form of a crystal of MURG. In practice, a MurG crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal, uranyl acetate or mercuric chloride, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used to construct three-dimensional structure of the enzyme. Blundel, T. L. and N. L. Johnson, Protein Crystallography, Academic Press (1976).

Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for MURG or MURG homologues or MURG mutants that have a root mean square deviation of protein backbone atoms (N, C.alpha., C and O) of less than 0.75 Å when superimposed--using backbone atoms--on the structure coordinates listed in Table 1, Table 2 or Table 3 shall be considered identical.

The term "unit cell" refers to a basic parallelepiped shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "molecular replacement" refers to a method that involves generating a preliminary model of a MurG crystal whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known (e.g., MURG coordinates from Table 1, 2, or 3) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final,

accurate structure of the unknown crystal. Lattman, E., "Use of the Rotation and Translation Functions", in Methods in Enzymology, 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, (1972). Using the structure coordinates of MURG provided by this invention, molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of MURG or of a different crystal form of MURG.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to the discovery of the three-dimensional structure of the crystalline form of the *E. coli* MurG protein, models of such three-dimensional structures, a method of structure based drug design using such structures, methods to identify ligands or compounds that interact or bind with such structures, the compounds identified by such methods, and the use of such compounds in therapeutic compositions.

More particularly, the present invention relates to novel crystals of *E. coli* MurG protein, methods of production of such crystals, three dimensional coordinates of MurG protein, MurG structures and models derived from the *E. coli* MurG structure, and uses of such structures and models to derive other MurG structures and in ligand discovery and drug design strategies.

The present invention also relates to three-dimensional structures and coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, structures and models of the binding sites, and uses of such structures and models to derive the binding sites of other MurG proteins and in drug design strategies.

Solely for ease of explanation, the description of the invention is divided into the following sections: (1) crystals of MurG protein; (2) methods of crystallization; (3) three-dimensional crystal coordinates and structure of *E. coli* MurG; (4) three-dimensional coordinates and structure of the donor nucleotide binding site of MurG; (5) coordinates and structure of the acceptor binding site of MurG; (5) three dimensional coordinates and structure of the membrane association site; (6) two dimensional and three dimensional images of the protein, α-carbon backbone, α-carbon backbone with conserved amino

acid residues, and binding sites; and (7) computer readable mediums comprising the three dimensional coordinates of the MurG protein, α-carbon backbone, α-carbon backbone with conserved amino acid residues, and binding sites; (8) images of structures of MurG protiensand binding sites; (9) models of MurG proteins and binding sites thereof and methods of using the structure of MurG to determine the structures of other MurG proteins and binding sites; (10) structure based drug design using models of MurG protein and binding site structures; (11) compounds derived from structure based drug design; and (12) therapeutic compositions using drugs designed from structure based drug design.

CRYSTALS

One embodiment of the present invention includes a composition comprising a MurG protein in a crystalline form (i.e., MurG crystals). As used herein, the terms (crystalline MurG" and "MurG crystal" both refer to crystallized MurG protein and are intended to be used interchangeably. More particularly, an embodiment of the present invention includes a composition comprising an *E. coli* MurG protein in a crystalline form. Preferably, a crystalline MurG is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 1. A MurG crystal of the present invention comprises any crystal structure and preferably precipitates as a triclinic crystal. Preferably, a composition of the present invention includes MurG crystal molecules arranged in a crystalline manner in a P1 space group with two molecules per assymmetric unit so as to form a unit cell of dimensions a=60.613 Å, b=66.356 Å, c=67.902 Å, α=64.294, β=83.520, γ=65.448. A preferred crystal of the present invention provides X-ray diffraction data for determination of atomic coordinates to a resolution of about 3.0 Å, preferably to about 2.4 Å, and more preferably to about 1.8 Å.

Another embodiment of the present invention includes crystalline MurG protein co-crystallized with a donor nucleotide or substrate or substrate analog. Preferably, a donor nucleotide is UDP or UDP-GlcNAc (UDP-N-acetylglucosamine) or an analog thereof. The substrate or substrate analog is preferably Lipid I or Lipid II, or analogs of Lipid I or Lipid II. More specifically, Lipid I and II analogs are as described in PCT/US99/02187, published as WO99/38958 and US Provisional Application Nos.

60/122,966 filed March 3, 1999 and 60/137,696 filed June 4, 1999, and International Application No. PCT/US00/05554 entitled "Bacterial transglycosylases: Assays for monitoring the activity using lipid II substrate analogs and methods for discovering antibiotics," all incorporated herein by reference in their entirety.

Included in the present invention, a variety of MurG proteins from numerous organisms can be used to prepare MurG crystals, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

In another embodiment of the present invention, the MurG proteins or fragments thereof, mutants or homologs are expressed in, for example, an *E. coli* host cell for use expressing sufficient quantities of sufficiently purified protein to form crystals. The present inventors have demonstrated that it is possible to express *Enterococcus. faecalis* MurG in *E. coli* cells – so the MurG proteins from many organisms can be cloned into expression vectors suitable for expression in *E. coli* cells. This would facilitate obtaining sufficient quanitites of isolated or purified MurG proteins. The expression of *E. faecalis* MurG protein in *E. coli* host cells is performed, for example, by expressing the *E. faecalis* MurG gene cloned into a pET21b expression vector and transformed into an *E. coli* host cell. The MurG protein is over-expressed with a C-terminal his tag (LEHHHHHH) which allows the protein to be purified using a His-tag affinity column. The protein is then crystallized and the atomic coordinates are determined using X-ray diffraction and methods known to those skilled in the art.

It is another embodiment of the present invention to provide for the construction and expression of chimeric MurG proteins to enable the crystallization and determination of the three dimensional coordinates of such chimeras. For example, if there are problems obtaining or crystallizing MurGs from other organisms, the present invention

provides information that makes it possible to make chimaeric proteins containing the donor or acceptor binding site from *E. coli* MurG and the corresponding acceptor or donor binding site from another organism. Chimaeric proteins could be easier to express, handle, or crystallize. For example, we have found that E. faecalis MurG is more difficult to solubilize that *E. coli* MurG (requiring more detergent). It is believed that the problems are related to the acceptor binding domain having a stronger affinity for the bacterial membranes. To overcome this problem, one can attach the donor binding domain of *E. faecalis* to the *E. coli* acceptor binding site and determine structure to see details of *E. faecalis* donor binding domain.

According to the present invention, crystalline MurG can be used to determine the ability of a chemical compound to bind to a MurG protein in a manner predicted by a structure based drug design method of the present invention. Preferably, a MurG crystal is soaked in a solution containing a chemical compound of the present invention. Binding of the chemical compound to the crystal is then determined by methods standard in the art. Thereby, the co-crystal of MurG and a compound of interest is determined.

METHODS OF CRYSTALLIZATION

The present invention includes a method for producing crystals of MurG proteins, comprising: combining MurG protein with a reservoir solution and inducing crystal formation to produce MurG crystals. Another embodiment of the present invention, a method for producing crystals of MurG protein comprises combining MurG protein with UDP-GlcNAc in a 1:3 ratio and with a reservoir solution and inducing crystal formation to produce MurG crystals.

Preferably, crystals of MurG are formed using a solution containing a range of MurG protein from about 1 mg/ml to about 20 mg/ml, more preferably above 5 mg/ml, limited only by the solubility of the protein, which may vary depending on the specific amino acid sequence.

A reservoir solution contains the buffer, the precipitant, and additives if necessary. A suitable reservoir buffer of the present invention comprises NaMES (2-[N-morpholino]ethanesulfonic acid, sodium salt) buffer, NaHEPES (N-[2-hydroxyethyl]piperazine-N'-[2-ethanesulfonic acid, sodium salt) buffer, Tris (tris[hydroxymethyl]aminomethane) buffer, and any buffer which has the PKa between

5.5 and 8.0. A suitable NaMES buffer solution has a pH range from about 5.6-6.5. Most preferably, the NaMES buffer has a pH of about 6.5. The precipitant comprises ammonium sulfate, saturated sodium and potassium tartrate and polyethylene glycol. A suitable concentration of ammonium sulfate can range from 0.8 M to 1.5 M. Most preferably, the ammonium sulfate concentration is about 0.96 M. A suitable additive comprises detergents like Triton X-100 and n-octyl-beta-glucoside. The concentration of Triton X-100 can range from 0.1% to 1%. Most preferably, the concentration of Triton X-100 is 0.4%.

In a preferred embodiment, MurG crystals are produced by a method comprising concentrating MurG protein in a buffer solution, mixing the protein concentrate with UDP-GlcNAc in a 1:3 molar ratio, mixing equal volumes of protein solution with a reservoir solution, and inducing crystal formation to produce MurG crystals.

In a particular embodiment of the invention, MurG crystals are produced by a method comprising concentrating MurG protein to 10 mg/ml in a buffer of 20 mM Tris-HCl, pH 7.9/150mM NaCl and 50 mM EDTA; mixing the protein concentrate with UDP-GlcNAc in a 1:3 molar ratio; mixing equal volumes of protein solution with a reservoir solution comprising (0.1 M NaMES, pH 6.5, 0.96 M $(NH_4)_2SO_4$, 0.4% TRITON® X-100, and 10 mM dithiolthreitol (DTT)), and inducing crystal formation using hanging drop vapor-diffusion.. This preferred method is described in greater detail in Example 1.

Supersaturated solutions of MurG protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of MurG protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, a MurG protein solution is combined with a reservoir solution of the present invention that will cause the MurG protein solution to become supersaturated and form MurG crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature in the range of from about 15°C to about 30°C, more preferably from about 20°C to about 25°C, and most preferably at a constant temperature of about 22°C.

In another preferred embodiment, the present invention includes a method to produce crystals of MurG protein comprising the steps of: (a) preparing an about 10

mg/ml solution of MurG protein in a Tris-HCl buffer, (b) mixing UDP-GlcNAc with the MurG protein solution in a 3:1 molar ratio, (c) dropping 2 µl droplet of this protein sample onto a coverslip, (d) adding an equal volume of reservoir solution to this droplet and inverting this over a well containing about 1 ml of the reservoir solution; and (e) incubating until crystals of MurG form.

Any isolated MurG protein can be used with the present method. An isolated MurG protein can be isolated from its natural milieu or produced using recombinant DNA technology (e.g., polymerase chain reaction (PCR) amplification, cloning) or chemical synthesis. To produce recombinant MurG protein, a nucleic acid molecule encoding a MurG protein can be inserted into any vector capable of expressing the nucleic acid in a host cell. Suitable and preferred nucleic acid molecules to include in recombinant vectors of the present invention are as disclosed herein. Such suitable and preferred nucleic acid molecules include numerous MurG encoding genes that have been isolated to date, and that will be isolated in the future. A preferred nucleic acid molecule of the present invention encodes a homologue of MurG. Homologues of MurG can be recognized by the presence of certain conserved amino acid residues or sequences.

A sequence alignment for six MurG sequences is shown in fig. 3A. Highlighted residues include those that are invariant or almost invariant across all MurG proteins. A nucleic acid molecule of the present invention can encode any portion of a MurG protein, preferably a full-length MurG protein or either of the two domains. A more preferred nucleic acid molecule to include in a recombinant vector, and particularly in a recombinant molecule, includes a nucleic acid molecule encoding a protein having the amino acid sequence represented by amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552,)67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640,

AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. Further, examples of nucleic acid molecules encoding MurG proteins have been deposited in NCBI, Genbank, and have Accession Nos. AL162758, AE002281, D90917, AF110367, AL139077, AJ242646, AE000520, AE000511, L42023, U00096, NC-000922, AE000783, AE000657, AE001348, AF099188, AR048673, AR048672, AF179611, AL022602, AL109663, X55034, AE000621, D10602, AE001670, X64259, Y13922, U10879, AE001535, AF068902, AJ235271, AE000118, AE001227, AE001176, U94707, Z95388, U32793, AE000727, D84504, Z99111, D10483,X52644, X52540, and L24773. These sequences are known and are publicly available. Further, as additional genomes and genes are sequenced, more MurG encoding nucleotide sequences will become available, and can be used in the present invention.

In specific embodiments of the invention, the protein sequence of *E. coli* MurG was reported in 1990 (Ikeda et al. Nucleic Acids Res. 1990, 19:4014; and Mengin-Lecreuix, D. et al., Nucleic Acids Res. 1990, 18:2810.). *E. coli* genomic DNA can be purified from *E. coli* or purchased from ATCC, or the gene for *E. coli* MurG is cloned into a plasmid can be obtained from numerous sources. Primers were designed to the portions of the gene corresponding to the N and C termini of the protein. The primers also encoded restriction enzyme sites outside the protein coding region. The gene sequence was amplified; the corresponding double stranded nucleic acid molecule was cut with appropriate restriction enzymes for cloning into a commercially available expression vector (pET expression vectors available from Novagen provide for numerous variations of MurG protein – wild-type or fusion proteins or proteins with affinity tags at N or C terminus. We have worked with several constructs but found that MurG with a His-tag at C-terminus crystallized best; the protein sequence contained an extra methionine at N-terminus and eight extra residues at C terminus, six of which were histidines. The vector used was pET21b. (as described in Ha et al. J. Am. Chem. Soc. 121, (1999) 8415-8426 hereby incorporated by reference in its entirety).

A recombinant vector of the present invention can be either RNA (probably not) or DNA, and typically includes, but is not limited to, a virus or plasmid. Any recombinant vector and host cell that provides for expression of a MurG protein

encoding mucleic acid sequence can be used in the present invention to express MurG protein for crystallization. Preferred vectors are engineered for high level expression in E. coli such as, but not limited to, pET vectors. We have found that over-expression of Murg from either *E. coli* or *E. faecalis* in *E. coli* cells is not toxic and, thus, this approach will work for other MurG proteins.

As used herein, an expression vector is a DNA vector that is capable of transforming a host cell and of affecting expression of a specified nucleic acid molecule. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including bacterial, fungal, and other microorganisms cells. Preferred expression vectors of the present invention direct expression in bacterial cells from a plasmid. A preferred recombinant molecule of the present invention comprises pET21b with E. coli MurG gene cloned into the Nde1 and Xho1 sites.

An expression vector of the present invention can be transformed into any suitable host cell to form a recombinant cell. A suitable host cell includes any cell capable of expressing a nucleic acid molecule inserted into the expression vector. For example, a procaryotic expression vector can be transformed into a bacterial host cell. If the expression vector contains a T7 promoter then a source of T7 RNA polymerase must be provided to induce expression. Some host cells contain the T7 RNA polymerase gene in a repressed state. Expression of T7 RNA polymerase can be induced with a chemical signal such as IPTG or heat. Alternatively, a source of T7 RNA polymerase can be introduced at the appropriate time by infection with a phage containing a copy of T7 RNA polymerase. A wide range of hosts strains can be infected with a suitable phage. Some host strains have been engineered to contain inducible copies of T7 RNA polymerase gene. Such host strains include BL21(DE3) and derivatives thereof. A preferred host strain of the present invention is BL21(DE3)pLysS or BL21(DE3)pLysE, which are commercially available from Novagen and can be readily transformed with a DNA plasmid vector containing a MurG gene under the control of the T7 promoter. As already stated above, a preferred vector is a pET vector, preferably containing a restriction enzyme site permitting cloning of the gene as a fusion containing a C-terminal his tag.

In a preferred embodiment, one method to isolate MurG protein useful for producing MurG crystals includes recovery of MurG protein having a C-terminal LEHHHHHH (His tag) sequence purified as described in Ha *et al.* (1999, J. Amer. Chem. Soc. 121:8415-8426). One of skill in the art is able to modify this procedure in order to purify other proteins can be produced as C-terminal histadine (his) tags. The purification conditions for specific MurG proteins will vary depending upon the particular characteristics of the proteins such as their isoelectric point, molecular weight, etc. It is known that the isoelectric points of different Murg homologues vary a bit, although they are generally relatively high. Also, some Murg homologues may be more hydrophobic than others, which will mean differences in amount of detergent necessary for purification. It is likely that all the Murg homologues can be purified over nickel affinity columns using the C-terminal his-tag as a handle. Those skilled in the art of protein purification will know how to modify purification parameters depending upon the protein characteristics, in order to purify the protein for crystallization.

STRUCTURE OF MURG PROTEIN

One embodiment of the present invention includes a model of a MurG protein, in which the model represents a three dimensional structure of a MurG protein. Another embodiment of the present invention includes the three dimensional structure of a MurG protein. A three dimensional structure of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 1. According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 1) to allow the three dimensional structure of another MurG protein to be modeled or calculated using the particular set of atomic coordinates defining the three dimensional configuration of the MurG protein. For example, but not meant to be a limitation, homology modeling can be done using the linear sequence of a different MurG and E. coli coordinates; molecular replacement can allow the solution of a different MurG structure using the *E. coli* MurG coordinates and experimental data such as x-ray diffraction pattern from a different MurG crystal. According to the present invention, a three dimensional structure of a

given portion or chain of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the α-carbon or C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that is actually represented by such atomic coordinates. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the common amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å.

In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the common amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the common amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the common amino acid side chains have the recited average RMSD value.

In more preferred embodiments of the present invention, a large number of different "rotamers" or "rotational isomers" of the MurG protein are encompassed by three dimensional structures of the invention in which the amino acid side chains are at a variety of positions in crystalline forms of the protein or for the protein in solution. Different rotamers refer to molecules of identical configuration may be distinguished as having different conformations after rotation about the various molecular bonds. Therefore, while the same or similar amino acids may be present, the exact location will vary depending upon the freedom of rotation of the bonds due to hydrogen bonding, and other molecular forces.

STRUCTURE OF THE α-CARBON BACKBONE OF MURG AND THE α-CARBON BACKBONE AND CONSERVED AMINO ACID RESIDUES

The present invention includes the three dimensional structure of the α-carbon or C-alpha backbone of a MurG protein, in particular the *E. coli* MurG protein. A three dimensional structure of the C-alpha backbone of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 2.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value. The C-alpha backbone of MurG proteins is expected to be more conserved than the location of the particular amino acid residue side chains.

The present invention also includes the three dimensional structure of the α-carbon or C-alpha backbone and conserved or invariant amino acid residue side chains of a MurG protein, in particular the *E. coli* MurG protein. A three dimensional structure of the C-alpha backbone and conserved amino acid residues of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 3. The conserved amino acids are highlighted in blue in Figure 3a and include G14, G15, G18, H19, G104, H124, E125, G190, G191, S192, G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a).

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the C-alpha backbone and conserved amino acid residue atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

STRUCTURE OF THE DONOR NUCLEOTIDE BINDING SITE OF MURG PROTEINS

An embodiment of the present invention includes the three dimensional structure of a donor nucleotide binding site of a MurG protein, in particular an *E. coli* MurG protein. A more preferred embodiment of the present invention includes a three dimensional structure of a donor nucleotide binding site of a MurG protein wherein the three dimensional structure of the donor nucleotide binding site substantially conforms to the atomic coordinates in Table 4. In a preferred embodiment, the donor nucleotide binding site is a UDP-GlcNAc binding site of a MurG protein.

As described in Example 1, the donor nucleotide binding site is located in the C-terminal domain (see Fig. 4a). This binding site is based on the comparison of β-glucosyltransferase (BGT) and *E. coli* MurG and based on experiments done in our laboratory showing that the isolated C domain binds to a UDP-hexose column (See Example 1). The atomic coordinates of Table 4 set forth the donor nucleotide binding site three dimensional structure without a donor nucleotide such as UDP-GlcNAc bound to the MurG protein.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a donor nucleotide binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 4) to allow the three dimensional structure of the donor nucleotide binding domain to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three dimensional configuration of the donor nucleotide binding site of a MurG protein. According to the present invention, a three dimensional structure of a given donor nucleotide binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG. Since the atomic coordinates of Table 4 were obtained from the *E. coli* MurG crystal protein without a donor nucleotide bound, there will be some variation from the atomic coordinates of the donor nucleotide binding site when a nucleotide is bound vs. unbound. Therefore, a structure "substantially conforming" to that represented by the atomic coordinates in Table 4, will include a structure obtained from co-crytallization of the protein with a donor nucleotide.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and more preferably less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that

substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved or invariant amino acid side chains located within the binding site. As used herein, the phrase "conserved amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins within the donor nucleotide binding site. The conserved amino acid residues of the donor nucleotide binding site have been identified as I125, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and the G loop found between residues numbered 190-195 having residues G190, G191, S192, G194, and A195. Some or all of these conserved residues are necessary for binding the nucleotide donor.

Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF THE ACCEPTOR BINDING SITE OF MURG PROTEIN

An embodiment of the present invention includes the three dimensional structure of an acceptor binding site of a MurG protein. A three dimensional structure of a acceptor binding site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 5. A more preferred embodiment of the present invention includes a three dimensional structure of an

acceptor binding site of a MurG protein wherein the three dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates Table 5.

According to the present invention, the use of the term "acceptors" refers to Lipid I and analogues thereof. For the purposes of obtaining co-crystals containing acceptor analogues bound to the acceptor binding site better, the analogues need not be functional acceptors in a MurG assay. In particular embodiments of the present invention, the acceptor is selected from the group consisting of, but not limited to Lipid I, and analogs of Lipid I (see compounds described in Ha et al., J. Amer. Chem. Soc. 1999, vol. 121:8415-26, incorporated by herein by reference in its entirety).

As described in Example 1, the acceptor binding site is located in the N-terminal domain of a MurG protein (see Fig. 3a and 4c). The acceptor binding site or domain is characterized by three highly conserved regions, two of which are glycine-rich loops (also referred to as "G loops") that face the cleft between the C-terminal and N-terminal domains. The conserved residues of the acceptor binding site comprise G14, G15, G18, H19, G104, H124, and E125 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and two conserved G loop structures.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of an acceptor binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 5) to allow the three dimensional structure of the acceptor binding site to be modeled or calculated (i.e., by homology modeling) using the particular set of atomic coordinates defining the three dimensional configuration of the acceptor binding site of a MurG protein. According to the present invention, a three dimensional structure of a given acceptor binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to the conserved or invariant amino acid side chains that are common to MurG proteins. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a

structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF A MEMBRANE ASSOCIATION SITE OF MurG PROTEIN

An embodiment of the present invention includes the three dimensional structure of a membrane association site of a MurG protein. A three dimensional structure of a membrane association site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 6. A more preferred embodiment of the present invention includes a three dimensional structure of an acceptor binding site of a MurG protein wherein the three dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates in Table 6.

According to the present invention, the use of the term "membrane association site" refers to the region of a MurG protein that associates with cytoplasmic surface of bacterial membranes where it performs the reaction of coupling a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG protein structure shows a hydrophobic patch consisting of residues I75, L79, F82, W85, and W116 in the N-domain. The membrane association site is where the MurG protein associates with the bacterial membranes, and that it is target for inhibitors if we find that a) we can bind to it with another molecule; b) we can disrupt membrane association by binding to it; or c) disrupting membrane association inhibits activity.

As described in Example 1, the membrane association site is located in the N-terminal domain of a MurG protein (see Fig. 4c). The location of the membrane association site is in close proximity to the acceptor binding site and membrane

association in this patch would bring the two M-terminal G-loops close to the membrane surface where the diphosphate portion of the acceptor is located.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a membrane association site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 6) to allow the three dimensional structure of the membrane association site to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three dimensional configuration of the membrane association site of a MurG protein. According to the present invention, a three dimensional structure of a given membrane association site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the structural elements in the site, and more preferably, less than about 1.3 Å for the structure elements in each site, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and more preferably, less than about 0.3 Å for the structural elements in each site. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of α-carbon backbone and conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved α-carbon backbone and conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less

than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the α-carbon backbone and conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the α-carbon backbone and conserved acid side chains have the recited average RMSD value, and most preferably, about 100% of the α-carbon and conserved amino acid side chains have the recited average RMSD value.

COMPUTER READABLE MEDIUM

Another embodiment of the present invention relates to a computer-readable medium encoded with a set three dimensional coordinates seleceted from the group consisting of the three dimensional coordinates represented in Table1, the three dimensional coordinates represented in Table 2, the three dimensional coordinates represented in Table 3, the three dimensional coordinates represented in Table 4, the three dimensional coordinates represented in Table 5, or the three dimensional coordinates represented in Table 6, wherein using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. Preferably, the three dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Yet another embodiment of the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates of a three dimensional structure which substantially conforms to the three dimensional coordinates represented in Table 1, wherein using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. In other embodiments, the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates of a three dimensional structure which substantially conforms to the three dimensional coordinates represented in Table 2, Table 3, Table 4, Table 5 or Table 6, wherein using a graphical display software program, the three dimensional

coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. Preferably, the three dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

IMAGES

One embodiment of the present invention relates to a two dimensional image of an *E. coli* MurG protein including those illustrated in Figures 3-4. Most of these figures were drawn with the MOLSCRIPT program. Preferably, the two dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Another embodiment of the present invention includes a three dimensional computer image of the three dimensional structure of a MurG protein, preferably the *E. coli* MurG protein. Suitable structures of which to produce three dimensional computer images are disclosed herein. Preferably, a computer image is created to a structure substantially conforming with the three dimensional coordinates represented in Table 1.

Another embodiment of the present invention includes an image of an MurG protein that is generated when a set of three dimensional coordinates comprising the three dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file as a three dimensional image. Suitable structures to image are disclosed herein. Preferably, the three dimensional structures are of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG. Most preferably, the MurG protein is the *E. coli* MurG protein described herein. A computer image of the present invention can be produced using any suitable software program, including, but not limited to, MOLSCRIPT 2.0 (Avatar Software AB, Helenebrgsgatan 21C, SE-11713, Stockholm, Sweden), the graphical display program O (Jones et al., Acta

Crystallography, vol. A47, p. 110, 1991), or the graphical display program GRASP. Suitable computer hardware useful for producing an image of the present invention are known to those of skill in the art. Preferred computer hardware includes a Silicon Graphics Workstation.

MODELS OF MURG PROTEINS AND BINDING SITES

According to the present invention, a three dimensional structure of the *E. coli* MurG protein and its binding sites of the present invention can be used to derive a model of the three dimensional structure of another MurG protein and its binding sites (i.e., a structure to be modeled). As used herein, a "structure" of a protein refers to the components and the manner of arrangement of the components to constitute a protein or binding site. Also, as used herein, the term "model" refers to a representation of a tangible medium of the three dimensional structure of a protein, polypeptide or peptide, or binding site of a protein. For example, a model can be a representation of the three dimensional structure in a electronic file, on a computer screen, on a piece of paper (i.e., on a two dimensional medium), and/or as a ball-and-stick figure. Physical three-dimensional models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, and Biosym Technologies, San Diego, CA. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Computer screen images and pictures of the model can be visualized in a number of formats including space-filling representations, α carbon traces, ribbon diagrams and electron density maps.

Suitable target MurG proteins and their associated binding sites to model using a method of the present invention include any MurG protein and binding sites that are at least in part structurally related to the *E. coli* MurG protein or its binding sites. A preferred target MurG structure that is at least in part structurally related includes a target MurG structure having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 36%, more preferably at least about 40%,

even more preferablye at least about 50%, more preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80%, and more preferably at least about 90% identical to an amino acid sequence of the *E. coli* MurG protein, across the full-length of the target MurG structure sequence when using, for example, a sequence alignment program such as DNAsis™ program (available from Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT) or the GCγ™ program (available from the "GCγ", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such alignment programs.

Preferred MurG proteins and their binding sites are set forth in the amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. The amino acid sequences are publicly available.

A variety of MurG proteins from numerous organisms can be used to prepare models of MurG proteins and binding sites, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus*

pneumoniae, *Synechocystis* sp. (strain PCC6803), *Thermotoga maritime*, and *Treponema pallidum*. It is noted that nucleotide and amino acid sequences for many of the above identified organisms are known and publicly available.

Preferred target MurG proteins and binding site structures to model also include, but are not limited to, derivatives of MurG proteins, such as a MurG protein having one or more amino acid residues substituted, deleted or added (referred to herein as MurG mutants), or proteins encoded by natural variants of a nucleic acid molecule encoding a MurG.

In another embodiment of the invention, the process of building a homology model for a protein is divided into the following steps:

(1) Determine which proteins are related to the model protein;

(2) Determine structurally conserved regions (SCRs);

(3) Align the amino acid sequence of the unknown protein with those of the reference protein(s) within the SCRs;

(4) Assign coordinates in the conserved regions;

(5) Predict conformations for the rest of the peptide chain, including loops between the SCRs and possibly the N- and C-termini;

(6) Search for the optimum side chain conformations for residues that differ from those in the reference proteins; and

(7) Use energy minimization and molecular dynamics to refine the molecular structure so that steric strain introduced during the model-building process can be relieved.

Published sequences are readily available through on-line databases on the Internet, such as SwissProt (http://www.expasy.ch/sprot/sprot-top.html). MurG specific and related sequences are obtained for use for building homology models by text-based or sequence similarity searching. SCRs for MurG is the entire protein, considering the E. coli MurG crystal structure is the only similar sequence with structural data. Alignment of the sequences using an appropriate alignment program and algorithm, such as Clustal W, allows appropriate assignment of the E. coli protein coordinates to a MurG sequence of unknown structure. The Modeler program performs the conformational predictions

for the peptide chain and side chains. Dynamics and minimization using an appropriate program and algorithm, such as Discover.

Modeler Description:

Modeler is an automated homology-modeling scheme designed to find the most probable three-dimensional structure of a protein, given its amino acid sequence and its alignment with related structures. It derives 3D protein models without the time consuming separate stages of core region identification and loop region building or searching that is inherent to manual homology modeling schemes. The related or reference protein structures are used to derive spatial restraints expressed as probability density functions (PDFs) for each of the restrained features of the model. As an example, the main chain conformation of a given residue in the model will be described by restraints that depend upon the residue type, the main chain conformation of equivalent residues in the reference proteins and the local sequence similarity. The probability distribution functions that are used in restraining the model structure are derived from correlations between structural features in a database of families of homologous proteins aligned on the basis of their 3D structure. These functions are used to restrain C-C distances, main chain N--O distances, main chain and side chain dihedral angles, etc. The individual restraints are assembled into a single molecular probability density function (MPDF). The three-dimensional protein model is then obtained by an optimization of this MPDF. The optimization procedure itself consists of a variable target function method (Braun and Go, 1985) with conjugate gradient minimization scheme followed by an optional restrained simulated annealing molecular dynamics scheme.

While several reference structures are used in the traditional homology model building process, only one set of coordinates can be used in any one peptide segment. Modeler is able to simultaneously incorporate structural data from one or more reference proteins. Structural features in the reference proteins are used to derive spatial restraints which in turn are used to generate model protein structures using conjugate gradient and simulated annealing optimization procedures.

Clustal W description:

Clustal W aligns multiple sequences using a progressive pairwise alignment algorithm. It first generates all possible pairwise alignments for a list of sequences and then builds the guide tree based on their pairwise sequence identity, aligning the sequences following the order of the guide tree.

Several unique features in Clustal W improve the sensitivity of the alignment of divergent protein sequences (Thompson et al, 1994a).

(1) Individual weights are assigned to each sequence in a partial alignment in order to downweight near-duplicate sequences and upweight the most divergent ones.

(2) Amino acid substitution matrices are varied at different alignment stages according to the divergence of the sequences to be aligned.

(3) Residue-specific gap penalties and locally reduced gap penalties in hydrophilic regions encourage new gaps in potential loop regions rather than regular secondary structure.

(4) Positions in early alignments, where gaps have been opened, receive locally reduced gap penalties to encourage the opening of new gaps at these positions.

Discover Description:

The Discover program performs energy minimization, template forcing, torsion forcing, and dynamic trajectories and calculates properties such as interaction energies, derivatives, mean square displacements, and vibrational frequencies. It provides tools for performing simulations under various conditions including constant temperature, constant pressure, constant stress, periodic boundaries, and fixed and restrained atoms.

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STRUCTURE BASED DRUG DESIGN

The present invention relates to the use of the crystal structure of the *E. coli* MurG protein represented by the atomic coordinates in Table 1 to make models of MurG proteins and binding sites thereof. The present invention also relates to the use of the crystal structure, α-carbon backbone, α-carbon backbone plus conserved amino acid residue side chains or binding sites of the *E. coli* MurG protein to construct models of these structures in other MurG proteins.

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or accessory binding site of MURG, in whole or in part.

On approach enabled by this invention, is to use the structure coordinates of MURG to design compounds that bind to the enzyme and alter the physical properties of

the compounds in different ways, e.g., solubility. For example, this invention enables the design of compounds that act as inhibitors of the MURG enzyme by binding to, all or a portion of, the active site of MURG.

A second design approach is to probe a MurG crystal with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate MURG inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each tpe of solvent molecule sticks. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their MURG inhibitor activity. Travis, J., Science, 262, p. 1374 (1993).

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to MURG, with MURG. Thus, the time-dependent analysis of structural changes in MURG during its interaction with other molecules is enabled. The reaction intermediates of MURG can also be deduced from the reaction product in co-complex with MURG. Such information is useful to design improved analogues of known MURG inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the MURG enzyme and MURG-inhibitor co-complex. This provides a novel route for designing MURG inhibitors with both high specificity and stability.

Another approach made possible and enabled by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the MURG enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng, E. C. et al., J. Coma. Chem., 13, pp. 505-524 (1992).

Because MURG may crystallize in more than one crystal form, the structure coordinates of MURG, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of MURG. They may also be used to solve the structure of MURG mutants, MURG co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of MURG.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of MURG, a MurG mutant, or a MurG co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of MURG, may be determined using the MURG structure coordinates of this invention as provided in Tables 1-6. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio.

In addition, in accordance with this invention, MURG mutants may be crystallized in co-complex with known MURG inhibitors. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type MURG. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between MURG and a chemical entity or compound.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 2-3 .ANG. resolution X-ray date to an R value of about 0.20 or less using computer software, such as X-PLOR (Yale University, .COPYRGT.1992, distributed by Molecular Simulations, Inc.). See, e.g., Blundel & Johnson, supra; Methods in Enzvmoloav, vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985). This information may thus be used to design, synthezie and optimize novel classes of MURG inhibitors.

The structure coordinates of MURG mutants provided in this invention also facilitate the identification of related proteins or enzymes analogous to MURG in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing UDP-glycosyltransferase mediated diseases.

The design of compounds that bind to or inhibit MURG according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with MURG. Non-covalent molecular interactions important in the association of MURG with its substrate include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with MURG. Although certain portions of the compound will not directly

participate in this association with MURG, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of MURG, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with MURG.

The potential inhibitory or binding effect of a chemical compound on MURG may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and MURG, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to MURG and inhibit using the assay of Walker et al. patents (cited supra). In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of MURG may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of MURG.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with MURG and more particularly with the individual binding pockets of the MURG donor nucleotide binding site, acceptor binding site or membrane association site. This process may begin by visual inspection of, for example, the binding sites on the computer screen based on the MURG coordinates in Tables 1-6. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within an individual binding pocket of MURG as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities, including but not limited to:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules" J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, Mass.

3. AUTODOCK (Goodsell, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing" Proteins: Structure. Function, and Genetics, 8, pp. 195-202 (1990)) (AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.).

4. DOCK (Kuntz, I. D. et al., "A Geometric Approach to Macromolecule-Ligand Interactions" J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of MURG. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include, but are not limited to:

1. CAVEAT (Bartlett, P. A. et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989)). CAVEAT is available from the University of California, Berkeley, Calif.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif.). This area is reviewed in Martin, Y. C., "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992)).

3. HOOK (available from Molecular Simulations, Burlington, Mass.).

Instead of proceeding to build a MurG inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other MURG binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include, but are not limited to:

1. LUDI (Bohm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. ComR. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, Calif.

2. LEGEND (Nishibata, Y. and A. Itai, Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, Mass.

3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to MURG may be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as a MurG-inhibitor must also preferably traverse a volume not overlapping that occupied by the active site when it is bound to the native substrate. An effective MURG inhibitor must preferably demonstrate a relatively small difference in

energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient MURG inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. MURG inhibitors may interact with the enzyme in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the inhibitor binds to the enzyme.

A compound designed or selected as binding to MURG may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the enzyme when the inhibitor is bound to MURG, preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include, but are not limited to: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. .COPYRIGHT.1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Francisco, .COPYRIGHT.1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. .COPYRIGHT.1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif. .COPYRIGHT.1994). These programs may be implemented, for instance, using a Silicon Graphics workstation, IRIS Octane or IBM RISC/6000 workstation. Other hardware systems and software packages will be known to those skilled in the art.

Once a MurG-binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted

chemical compounds may then be analyzed for efficiency of fit to MURG by the same computer methods described in detail, above.

COMPOUNDS AND COMPOSITIONS COMPRISING COMPOUNDS DERIVED FROM STRUCTURE BASED DRUG DESIGN

One embodiment of the present invention is a compound that is capable of binding to a MurG protein, inhibiting the activity of a MurG protein, or stimulating the activity of a MurG protein. Suitable inhibitory compounds of the present invention can: (1) inhibit (i.e., prevent or block) the activity of MurG enzyme by binding to a MurG donor nucleotide binding site and interfering with the binding of the donor nucleotide molecule; (2) inhibit the activity of MurG enzyme by binding to the MurG acceptor binding site and interfering with the binding of the acceptor molecule; (3) inhibit the activity of a MurG enzyme by binding to the membrane association site and interfering with the association of the protein with the bacterial membrane and/or acceptor molecule.

Another embodiment of the present invention is a compound that is capable of stimulating MurG activity. Suitable stimulatory compounds of the present invention can stimulate the activity of a MurG enzyme by binding to the protein at a binding site and causing an increase in enzymatic activity, for example, by increasing the enzymes affinity to bind a donor nucleotide, an acceptor molecule or improve the enzymes stability or increasing the binding affinity of a molecule to MurG.

Such compounds that bind to, inhibit or stimulate activity of a MurG protein include, for example, compounds that mimic donor nucleotide molecules. In preferred embodiments, the compound includes, for example, pyrimidine nucleoside analogues. In yet another preferred embodiment, the compounds include compounds comprising a pyrimidine nucleoside with a substituent containing at least one heteroatom attached to the C5 hydroxyl. In more particular embodiments, pyrimidine derivatives make complementary hydrogen bonding contacts to the amide backbone segment containing Ile 245 and also contact glutamate 269.

Another embodiment of the present invention is a compound that binds to the acceptor binding site of the MurG protein, hereinafter referred to a acceptor analogs. An acceptor analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the acceptor binding site of a MurG protein. An acceptor analog, for example,

is a compound that mimics the natural acceptor molecule, Lipid I. Examples of such acceptor analogs are set forth in Ha et al., J. Amer. Chem. Soc. 1999, and PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, incorporated herein by reference.

Another embodiment of the present invention is a compound that binds to the MurG protein, that are enzyme product analogs, hereinafter referred to as Lipid II analogs. A Lipid II analog refers to a compound that interacts with (i.e. , binds to, associates with, modifies) the acceptor binding site of a Mur G protein which mimics the product of the transglycosylase reaction.

Inhibitory and stimulatory compounds of the present invention can be identified by various means known to those of skill in the art. For example, binding of an inhibitory compound to, or otherwise interaction with, a MurG protein, can be determined with MurG in solution, for example, using assays described in PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, and PCT/US00/05554 , U.S. Provisional Application Nos. 60/122,966 and 60/137,696, incorporated herein by reference.

According to the present invention, suitable compounds of the present invention include peptides or other organic molecules, and inorganic molecules. Suitable organic molecules include small organic molecules. Preferably, a compound of the present invention is not harmful (i.e., toxic) to an animal when administered to an animal.

Compounds of the present invention also can be identified using structure based drug design techniques known to those skilled in the art and described herein above.

Also according to the present invention, compounds are suitable for use in the inhibition of bacterial or microbial growth in an animal, and for example, function as an antibiotic for treatment of bacterial infections in animals.

The present invention also includes compositions comprising compounds of the present invention that inhibit or stimulate MurG activity which function as antibiotics or antimicrobial agents in animals. Compositions of the present invention can be used therapeutically or diagnostically in an animal. Compositions of the present invention comprises at least one compound of the present invention. In a preferred embodiment, compositions of the present invention further comprise a carrier. More particularly, a suitable carrier is a pharmaceutically acceptable carrier known to those skilled in the art.

TABLE 1- ATOMIC COORDINATES OF E. COLI MURG PROTEIN

REMARK coordinates from minimization refinementREMARK refinement resolution: 40.0 - 1.9 AREMARK starting r= 0.2200 free_r= 0.2466REMARK final r= 0.2200 free_r= 0.2466REMARK rmsd bonds= 0.005558 rmsd angles= 1.29505REMARK wa= 1.08391REMARK target= mlf cycles= 1 steps= 30REMARK sg= P1 a= 60.613 b= 66.356 c= 67.902 alpha= 64.294 beta= 83.520 gamma= 65.448REMARK parameter file 1 :
CNS_TOPPAR:protein_rep.paramREMARK parameter file 2 :
CNS_TOPPAR:water_rep.paramREMARK parameter file 3 :
CNS_TOPPAR:ion.paramREMARK molecular structure file: gen.mtfREMARK input coordinates: gen.pdbREMARK reflection file= native.cvREMARK ncs= noneREMARK B-correction resolution: 6.0 - 1.9REMARK initial B-factor correction applied to fobs :REMARK B11= 0.747 B22= 2.098 B33= -2.845REMARK B12= -1.847 B13= -3.752 B23= 6.401REMARK B-factor correction applied to coordinate array B: 0.038REMARK bulk solvent: density level= 0.351665 e/A^3, B-factor= 43.8282 A^2REMARK reflections with |Fobs|/sigma_F < 2.0 rejectedREMARK reflections with |Fobs| > 10000 * rms(Fobs) rejectedREMARK theoretical total number of refl. in resol. range:68102 (100.0%)REMARK number of unobserved reflections (no entry or |F|=0):2825(4.1%) REMARK number of reflections rejected: 3288 (4.8 %)REMARK total number of reflections used: 61989 91.0%)REMARK number of reflections in working set: 55765 (81.9%)REMARK number of reflections in test set: 6224 (9.1%)CRYST1 60.613 66.356 67.902 64.29 83.52 65.45 P 1
REMARK FILENAME="minimize5.pdb"REMARK DATE:14-Jan-00 15:25:36 created by user: shaREMARK VERSION: 0.5

ATOM	1	CB	LYS	A	7	0.142	3.434	35.023	1.00	43.02	AAAA
ATOM	2	CG	LYS	A	7	1.076	4.457	35.641	1.00	46.34	AAAA
ATOM	3	CD	LYS	A	7	0.452	5.841	35.634	1.00	47.39	AAAA
ATOM	4	CE	LYS	A	7	1.345	6.846	36.332	1.00	48.65	AAAA
ATOM	5	NZ	LYS	A	7	0.780	8.221	36.276	1.00	51.04	AAAA
ATOM	6	C	LYS	A	7	-2.239	2.733	34.833	1.00	39.64	AAAA
ATOM	7	O	LYS	A	7	-2.050	1.717	34.160	1.00	39.64	AAAA
ATOM	8	N	LYS	A	7	-0.974	2.320	36.947	1.00	42.05	AAAA
ATOM	9	CA	LYS	A	7	-1.170	3.245	35.788	1.00	41.31	AAAA
ATOM	10	N	ARG	A	8	-3.357	3.451	34.773	1.00	37.24	AAAA
ATOM	11	CA	ARG	A	8	-4.469	3.076	33.906	1.00	34.91	AAAA
ATOM	12	CB	ARG	A	8	-5.782	3.109	34.686	1.00	36.65	AAAA
ATOM	13	CG	ARG	A	8	-5.950	2.017	35.721	1.00	39.89	AAAA
ATOM	14	CD	ARG	A	8	-7.323	2.124	36.356	1.00	42.12	AAAA
ATOM	15	NE	ARG	A	8	-7.663	0.960	37.163	1.00	45.03	AAAA
ATOM	16	CZ	ARG	A	8	-7.031	0.610	38.279	1.00	46.29	AAAA
ATOM	17	NH1	ARG	A	8	-6.015	1.337	38.725	1.00	46.88	AAAA
ATOM	18	NH2	ARG	A	8	-7.420	-0.466	38.952	1.00	47.41	AAAA
ATOM	19	C	ARG	A	8	-4.584	3.999	32.696	1.00	32.27	AAAA
ATOM	20	O	ARG	A	8	-4.602	5.224	32.832	1.00	31.60	AAAA
ATOM	21	N	LEU	A	9	-4.663	3.403	31.512	1.00	29.57	AAAA
ATOM	22	CA	LEU	A	9	-4.792	4.171	30.283	1.00	27.45	AAAA
ATOM	23	CB	LEU	A	9	-3.581	3.954	29.362	1.00	26.31	AAAA
ATOM	24	CG	LEU	A	9	-3.752	4.466	27.916	1.00	25.77	AAAA
ATOM	25	CD1	LEU	A	9	-3.670	5.985	27.895	1.00	24.31	AAAA

ATOM	26	CD2	LEU	A	9	-2.679	3.870	26.993	1.00	26.22	AAAA
ATOM	27	C	LEU	A	9	-6.038	3.762	29.523	1.00	25.97	AAAA
ATOM	28	O	LEU	A	9	-6.397	2.587	29.485	1.00	25.57	AAAA
ATOM	29	N	MET	A	10	-6.713	4.738	28.928	1.00	25.37	AAAA
ATOM	30	CA	MET	A	10	-7.866	4.429	28.101	1.00	24.70	AAAA
ATOM	31	CB	MET	A	10	-9.142	5.101	28.612	1.00	25.60	AAAA
ATOM	32	CG	MET	A	10	-10.323	4.873	27.675	1.00	25.77	AAAA
ATOM	33	SD	MET	A	10	-11.916	4.958	28.492	1.00	26.63	AAAA
ATOM	34	CE	MET	A	10	-12.197	3.222	28.862	1.00	25.72	AAAA
ATOM	35	C	MET	A	10	-7.528	4.943	26.715	1.00	23.31	AAAA
ATOM	36	O	MET	A	10	-7.198	6.116	26.544	1.00	24.02	AAAA
ATOM	37	N	VAL	A	11	-7.574	4.059	25.727	1.00	22.25	AAAA
ATOM	38	CA	VAL	A	11	-7.278	4.461	24.359	1.00	22.34	AAAA
ATOM	39	CB	VAL	A	11	-6.444	3.386	23.624	1.00	22.75	AAAA
ATOM	40	CG1	VAL	A	11	-6.256	3.768	22.158	1.00	20.51	AAAA
ATOM	41	CG2	VAL	A	11	-5.082	3.239	24.310	1.00	21.75	AAAA
ATOM	42	C	VAL	A	11	-8.612	4.654	23.646	1.00	22.94	AAAA
ATOM	43	O	VAL	A	11	-9.525	3.843	23.804	1.00	23.37	AAAA
ATOM	44	N	MET	A	12	-8.722	5.734	22.878	1.00	22.18	AAAA
ATOM	45	CA	MET	A	12	-9.949	6.034	22.146	1.00	23.10	AAAA
ATOM	46	CB	MET	A	12	-10.496	7.399	22.589	1.00	22.78	AAAA
ATOM	47	CG	MET	A	12	-10.359	7.655	24.096	1.00	23.92	AAAA
ATOM	48	SD	MET	A	12	-10.955	9.279	24.657	1.00	25.51	AAAA
ATOM	49	CE	MET	A	12	-9.641	10.349	24.162	1.00	22.79	AAAA
ATOM	50	C	MET	A	12	-9.582	6.072	20.673	1.00	22.97	AAAA
ATOM	51	O	MET	A	12	-8.917	6.997	20.226	1.00	21.16	AAAA
ATOM	52	N	ALA	A	13	-9.992	5.057	19.921	1.00	26.97	AAAA
ATOM	53	CA	ALA	A	13	-9.665	5.008	18.498	1.00	30.88	AAAA
ATOM	54	CB	ALA	A	13	-8.381	4.212	18.288	1.00	31.18	AAAA
ATOM	55	C	ALA	A	13	-10.813	4.412	17.685	1.00	34.35	AAAA
ATOM	56	O	ALA	A	13	-11.328	3.335	18.006	1.00	35.86	AAAA
ATOM	57	N	GLY	A	14	-11.176	5.127	16.622	1.00	37.37	AAAA
ATOM	58	CA	GLY	A	14	-12.287	4.762	15.757	1.00	40.54	AAAA
ATOM	59	C	GLY	A	14	-12.239	3.583	14.808	1.00	41.52	AAAA
ATOM	60	O	GLY	A	14	-11.267	2.831	14.755	1.00	43.26	AAAA
ATOM	61	N	GLY	A	15	-13.322	3.451	14.042	1.00	42.70	AAAA
ATOM	62	CA	GLY	A	15	-13.491	2.363	13.094	1.00	43.13	AAAA
ATOM	63	C	GLY	A	15	-12.660	2.286	11.825	1.00	43.41	AAAA
ATOM	64	O	GLY	A	15	-13.212	2.187	10.730	1.00	44.39	AAAA
ATOM	65	N	THR	A	16	-11.340	2.333	11.966	1.00	43.38	AAAA
ATOM	66	CA	THR	A	16	-10.426	2.204	10.833	1.00	43.22	AAAA
ATOM	67	CB	THR	A	16	-10.120	3.551	10.110	1.00	44.23	AAAA
ATOM	68	OG1	THR	A	16	-9.302	4.375	10.949	1.00	44.41	AAAA
ATOM	69	CG2	THR	A	16	-11.404	4.286	9.754	1.00	43.74	AAAA
ATOM	70	C	THR	A	16	-9.118	1.679	11.402	1.00	43.06	AAAA
ATOM	71	O	THR	A	16	-8.728	2.042	12.517	1.00	42.99	AAAA
ATOM	72	N	GLY	A	17	-8.453	0.810	10.649	1.00	41.81	AAAA
ATOM	73	CA	GLY	A	17	-7.190	0.268	11.109	1.00	40.71	AAAA
ATOM	74	C	GLY	A	17	-6.202	1.401	11.275	1.00	39.54	AAAA
ATOM	75	O	GLY	A	17	-5.275	1.330	12.085	1.00	39.73	AAAA
ATOM	76	N	GLY	A	18	-6.413	2.460	10.500	1.00	37.79	AAAA
ATOM	77	CA	GLY	A	18	-5.539	3.611	10.572	1.00	35.68	AAAA
ATOM	78	C	GLY	A	18	-5.394	4.116	11.994	1.00	34.88	AAAA
ATOM	79	O	GLY	A	18	-4.285	4.441	12.427	1.00	35.21	AAAA
ATOM	80	N	HIS	A	19	-6.503	4.186	12.728	1.00	32.89	AAAA
ATOM	81	CA	HIS	A	19	-6.454	4.664	14.110	1.00	32.14	AAAA
ATOM	82	CB	HIS	A	19	-7.759	5.371	14.504	1.00	30.28	AAAA
ATOM	83	CG	HIS	A	19	-8.150	6.504	13.605	1.00	28.85	AAAA
ATOM	84	CD2	HIS	A	19	-9.336	6.808	13.027	1.00	27.83	AAAA
ATOM	85	ND1	HIS	A	19	-7.288	7.524	13.265	1.00	28.68	AAAA
ATOM	86	CE1	HIS	A	19	-7.926	8.407	12.517	1.00	28.09	AAAA
ATOM	87	NE2	HIS	A	19	-9.170	7.996	12.358	1.00	27.45	AAAA
ATOM	88	C	HIS	A	19	-6.229	3.533	15.108	1.00	31.91	AAAA
ATOM	89	O	HIS	A	19	-5.480	3.684	16.072	1.00	31.76	AAAA
ATOM	90	N	VAL	A	20	-6.895	2.407	14.881	1.00	31.82	AAAA
ATOM	91	CA	VAL	A	20	-6.813	1.271	15.788	1.00	33.08	AAAA

ATOM	92	CB	VAL	A	20	-7.875	0.215	15.430	1.00	33.31	AAAA
ATOM	93	CG1	VAL	A	20	-7.766	-0.982	16.361	1.00	33.91	AAAA
ATOM	94	CG2	VAL	A	20	-9.260	0.830	15.540	1.00	34.25	AAAA
ATOM	95	C	VAL	A	20	-5.452	0.587	15.898	1.00	33.31	AAAA
ATOM	96	O	VAL	A	20	-4.977	0.337	17.008	1.00	32.99	AAAA
ATOM	97	N	PHE	A	21	-4.823	0.288	14.765	1.00	33.64	AAAA
ATOM	98	CA	PHE	A	21	-3.526	-0.385	14.794	1.00	33.68	AAAA
ATOM	99	CB	PHE	A	21	-3.020	-0.648	13.368	1.00	35.58	AAAA
ATOM	100	CG	PHE	A	21	-3.900	-1.578	12.577	1.00	39.10	AAAA
ATOM	101	CD1	PHE	A	21	-4.463	-2.701	13.174	1.00	40.50	AAAA
ATOM	102	CD2	PHE	A	21	-4.157	-1.338	11.232	1.00	41.05	AAAA
ATOM	103	CE1	PHE	A	21	-5.271	-3.572	12.446	1.00	41.55	AAAA
ATOM	104	CE2	PHE	A	21	-4.964	-2.205	10.492	1.00	41.86	AAAA
ATOM	105	CZ	PHE	A	21	-5.521	-3.323	11.103	1.00	42.12	AAAA
ATOM	106	C	PHE	A	21	-2.456	0.350	15.605	1.00	32.04	AAAA
ATOM	107	O	PHE	A	21	-1.789	-0.257	16.443	1.00	31.30	AAAA
ATOM	108	N	PRO	A	22	-2.277	1.662	15.375	1.00	31.37	AAAA
ATOM	109	CD	PRO	A	22	-2.939	2.544	14.400	1.00	31.41	AAAA
ATOM	110	CA	PRO	A	22	-1.259	2.396	16.139	1.00	30.01	AAAA
ATOM	111	CB	PRO	A	22	-1.301	3.799	15.536	1.00	30.97	AAAA
ATOM	112	CG	PRO	A	22	-1.892	3.592	14.175	1.00	31.19	AAAA
ATOM	113	C	PRO	A	22	-1.620	2.411	17.624	1.00	29.31	AAAA
ATOM	114	O	PRO	A	22	-0.749	2.366	18.489	1.00	27.42	AAAA
ATOM	115	N	GLY	A	23	-2.918	2.483	17.903	1.00	28.99	AAAA
ATOM	116	CA	GLY	A	23	-3.380	2.492	19.277	1.00	28.59	AAAA
ATOM	117	C	GLY	A	23	-3.035	1.196	19.990	1.00	29.00	AAAA
ATOM	118	O	GLY	A	23	-2.649	1.205	21.160	1.00	28.48	AAAA
ATOM	119	N	LEU	A	24	-3.168	0.078	19.282	1.00	28.08	AAAA
ATOM	120	CA	LEU	A	24	-2.863	-1.227	19.859	1.00	28.39	AAAA
ATOM	121	CB	LEU	A	24	-3.306	-2.347	18.913	1.00	28.16	AAAA
ATOM	122	CG	LEU	A	24	-4.811	-2.605	18.843	1.00	28.45	AAAA
ATOM	123	CD1	LEU	A	24	-5.117	-3.583	17.714	1.00	29.25	AAAA
ATOM	124	CD2	LEU	A	24	-5.291	-3.158	20.181	1.00	29.35	AAAA
ATOM	125	C	LEU	A	24	-1.373	-1.350	20.147	1.00	28.37	AAAA
ATOM	126	O	LEU	A	24	-0.966	-1.986	21.126	1.00	28.60	AAAA
ATOM	127	N	ALA	A	25	-0.555	-0.743	19.296	1.00	27.77	AAAA
ATOM	128	CA	ALA	A	25	0.887	-0.795	19.497	1.00	28.98	AAAA
ATOM	129	CB	ALA	A	25	1.616	-0.142	18.321	1.00	27.53	AAAA
ATOM	130	C	ALA	A	25	1.256	-0.093	20.800	1.00	29.10	AAAA
ATOM	131	O	ALA	A	25	2.035	-0.618	21.595	1.00	29.49	AAAA
ATOM	132	N	VAL	A	26	0.694	1.094	21.020	1.00	28.82	AAAA
ATOM	133	CA	VAL	A	26	0.982	1.853	22.233	1.00	28.94	AAAA
ATOM	134	CB	VAL	A	26	0.400	3.290	22.157	1.00	29.74	AAAA
ATOM	135	CG1	VAL	A	26	0.691	4.049	23.454	1.00	29.76	AAAA
ATOM	136	CG2	VAL	A	26	1.009	4.026	20.981	1.00	29.14	AAAA
ATOM	137	C	VAL	A	26	0.409	1.131	23.450	1.00	29.18	AAAA
ATOM	138	O	VAL	A	26	1.020	1.118	24.518	1.00	29.62	AAAA
ATOM	139	N	ALA	A	27	-0.757	0.518	23.286	1.00	27.98	AAAA
ATOM	140	CA	ALA	A	27	-1.371	-0.215	24.382	1.00	29.32	AAAA
ATOM	141	CB	ALA	A	27	-2.719	-0.755	23.950	1.00	28.32	AAAA
ATOM	142	C	ALA	A	27	-0.462	-1.372	24.840	1.00	30.04	AAAA
ATOM	143	O	ALA	A	27	-0.084	-1.454	26.015	1.00	29.89	AAAA
ATOM	144	N	HIS	A	28	-0.120	-2.259	23.907	1.00	30.92	AAAA
ATOM	145	CA	HIS	A	28	0.734	-3.413	24.201	1.00	30.62	AAAA
ATOM	146	CB	HIS	A	28	1.024	-4.214	22.924	1.00	30.20	AAAA
ATOM	147	CG	HIS	A	28	-0.112	-5.080	22.483	1.00	31.65	AAAA
ATOM	148	CD2	HIS	A	28	-0.764	-5.162	21.299	1.00	31.33	AAAA
ATOM	149	ND1	HIS	A	28	-0.717	-5.996	23.319	1.00	31.81	AAAA
ATOM	150	CE1	HIS	A	28	-1.696	-6.600	22.670	1.00	32.38	AAAA
ATOM	151	NE2	HIS	A	28	-1.747	-6.112	21.443	1.00	32.85	AAAA
ATOM	152	C	HIS	A	28	2.054	-2.989	24.823	1.00	30.90	AAAA
ATOM	153	O	HIS	A	28	2.537	-3.601	25.779	1.00	30.92	AAAA
ATOM	154	N	HIS	A	29	2.636	-1.939	24.263	1.00	30.28	AAAA
ATOM	155	CA	HIS	A	29	3.899	-1.415	24.742	1.00	30.76	AAAA
ATOM	156	CB	HIS	A	29	4.276	-0.195	23.911	1.00	31.40	AAAA
ATOM	157	CG	HIS	A	29	5.679	0.274	24.122	1.00	33.14	AAAA

ATOM	158	CD2	HIS	A	29	6.188	1.226	24.939	1.00	33.77	AAAA
ATOM	159	ND1	HIS	A	29	6.748	-0.240	23.420	1.00	34.47	AAAA
ATOM	160	CE1	HIS	A	29	7.855	0.381	23.791	1.00	34.76	AAAA
ATOM	161	NE2	HIS	A	29	7.542	1.275	24.711	1.00	34.09	AAAA
ATOM	162	C	HIS	A	29	3.835	-1.032	26.227	1.00	31.63	AAAA
ATOM	163	O	HIS	A	29	4.763	-1.315	26.990	1.00	30.76	AAAA
ATOM	164	N	LEU	A	30	2.744	-0.388	26.638	1.00	29.72	AAAA
ATOM	165	CA	LEU	A	30	2.603	0.035	28.028	1.00	30.08	AAAA
ATOM	166	CB	LEU	A	30	1.631	1.225	28.126	1.00	29.45	AAAA
ATOM	167	CG	LEU	A	30	2.107	2.503	27.420	1.00	28.69	AAAA
ATOM	168	CD1	LEU	A	30	1.026	3.587	27.477	1.00	27.76	AAAA
ATOM	169	CD2	LEU	A	30	3.383	2.998	28.075	1.00	28.99	AAAA
ATOM	170	C	LEU	A	30	2.153	-1.096	28.950	1.00	30.55	AAAA
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ATOM	174	CB	MET	A	31	-0.118	-3.999	28.494	1.00	34.12	AAAA
ATOM	175	CG	MET	A	31	-1.452	-3.341	28.249	1.00	34.98	AAAA
ATOM	176	SD	MET	A	31	-2.618	-4.475	27.485	1.00	38.51	AAAA
ATOM	177	CE	MET	A	31	-2.086	-4.401	25.803	1.00	37.49	AAAA
ATOM	178	C	MET	A	31	2.078	-3.987	29.664	1.00	35.03	AAAA
ATOM	179	O	MET	A	31	2.101	-4.548	30.758	1.00	36.09	AAAA
ATOM	180	N	ALA	A	32	3.062	-4.085	28.776	1.00	35.62	AAAA
ATOM	181	CA	ALA	A	32	4.262	-4.871	29.044	1.00	37.61	AAAA
ATOM	182	CB	ALA	A	32	5.049	-5.087	27.755	1.00	37.79	AAAA
ATOM	183	C	ALA	A	32	5.133	-4.158	30.070	1.00	38.72	AAAA
ATOM	184	O	ALA	A	32	6.223	-4.621	30.409	1.00	39.48	AAAA
ATOM	185	N	GLN	A	33	4.654	-3.022	30.560	1.00	38.28	AAAA
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ATOM	188	CG	GLN	A	33	6.856	-1.210	29.791	1.00	42.76	AAAA
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ATOM	190	OE1	GLN	A	33	7.803	0.975	29.717	1.00	46.28	AAAA
ATOM	191	NE2	GLN	A	33	7.002	0.131	27.795	1.00	44.60	AAAA
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ATOM	193	O	GLN	A	33	4.822	-1.075	33.532	1.00	37.34	AAAA
ATOM	194	N	GLY	A	34	3.585	-2.877	33.000	1.00	35.86	AAAA
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ATOM	196	C	GLY	A	34	1.461	-1.951	34.008	1.00	34.34	AAAA
ATOM	197	O	GLY	A	34	0.611	-1.974	34.897	1.00	33.67	AAAA
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ATOM	199	CA	TRP	A	35	0.121	-0.435	32.661	1.00	33.63	AAAA
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ATOM	203	CE2	TRP	A	35	1.840	3.897	31.957	1.00	36.13	AAAA
ATOM	204	CE3	TRP	A	35	-0.499	3.705	31.350	1.00	37.33	AAAA
ATOM	205	CD1	TRP	A	35	2.469	1.759	32.099	1.00	35.78	AAAA
ATOM	206	NE1	TRP	A	35	2.893	3.062	32.221	1.00	34.49	AAAA
ATOM	207	CZ2	TRP	A	35	1.776	5.293	31.955	1.00	37.71	AAAA
ATOM	208	CZ3	TRP	A	35	-0.563	5.095	31.348	1.00	37.99	AAAA
ATOM	209	CH2	TRP	A	35	0.570	5.874	31.650	1.00	38.17	AAAA
ATOM	210	C	TRP	A	35	-1.153	-1.228	32.402	1.00	33.77	AAAA
ATOM	211	O	TRP	A	35	-1.136	-2.282	31.763	1.00	32.95	AAAA
ATOM	212	N	GLN	A	36	-2.261	-0.704	32.912	1.00	32.90	AAAA
ATOM	213	CA	GLN	A	36	-3.567	-1.301	32.696	1.00	33.08	AAAA
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ATOM	215	CG	GLN	A	36	-4.240	-2.228	34.992	1.00	38.58	AAAA
ATOM	216	CD	GLN	A	36	-5.272	-2.143	36.103	1.00	40.36	AAAA
ATOM	217	OE1	GLN	A	36	-5.295	-1.186	36.874	1.00	42.12	AAAA
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ATOM	219	C	GLN	A	36	-4.160	-0.482	31.552	1.00	32.42	AAAA
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ATOM	222	CA	VAL	A	37	-5.276	-0.456	29.403	1.00	31.91	AAAA
ATOM	223	CB	VAL	A	37	-4.436	-0.656	28.123	1.00	32.46	AAAA

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ATOM	225	CG2	VAL	A	37	-2.994	-0.269	28.379	1.00	31.40	AAAA
ATOM	226	C	VAL	A	37	-6.693	-0.917	29.118	1.00	32.15	AAAA
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ATOM	239	N	TRP	A	39	-10.119	0.072	26.332	1.00	28.69	AAAA
ATOM	240	CA	TRP	A	39	-10.414	0.729	25.071	1.00	28.19	AAAA
ATOM	241	CB	TRP	A	39	-10.321	-0.305	23.939	1.00	29.84	AAAA
ATOM	242	CG	TRP	A	39	-10.046	0.269	22.583	1.00	33.23	AAAA
ATOM	243	CD2	TRP	A	39	-8.774	0.339	21.919	1.00	33.62	AAAA
ATOM	244	CE2	TRP	A	39	-8.995	0.945	20.661	1.00	34.00	AAAA
ATOM	245	CE3	TRP	A	39	-7.470	-0.052	22.261	1.00	33.80	AAAA
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ATOM	247	NE1	TRP	A	39	-10.332	1.230	20.573	1.00	33.43	AAAA
ATOM	248	CZ2	TRP	A	39	-7.960	1.171	19.743	1.00	34.56	AAAA
ATOM	249	CZ3	TRP	A	39	-6.442	0.171	21.350	1.00	35.28	AAAA
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ATOM	254	CA	LEU	A	40	-13.197	3.159	24.130	1.00	23.18	AAAA
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ATOM	257	CD1	LEU	A	40	-15.314	4.801	25.675	1.00	21.21	AAAA
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ATOM	260	O	LEU	A	40	-12.718	3.721	21.854	1.00	22.99	AAAA
ATOM	261	N	GLY	A	41	-14.608	2.580	22.232	1.00	25.02	AAAA
ATOM	262	CA	GLY	A	41	-14.946	2.553	20.821	1.00	25.95	AAAA
ATOM	263	C	GLY	A	41	-16.426	2.332	20.594	1.00	28.01	AAAA
ATOM	264	O	GLY	A	41	-17.234	2.555	21.494	1.00	28.82	AAAA
ATOM	265	N	THR	A	42	-16.783	1.884	19.395	1.00	29.77	AAAA
ATOM	266	CA	THR	A	42	-18.185	1.641	19.059	1.00	31.41	AAAA
ATOM	267	CB	THR	A	42	-18.603	2.497	17.855	1.00	32.12	AAAA
ATOM	268	OG1	THR	A	42	-18.293	3.871	18.119	1.00	34.95	AAAA
ATOM	269	CG2	THR	A	42	-20.098	2.367	17.611	1.00	34.55	AAAA
ATOM	270	C	THR	A	42	-18.458	0.168	18.741	1.00	32.23	AAAA
ATOM	271	O	THR	A	42	-17.721	-0.463	17.986	1.00	29.57	AAAA
ATOM	272	N	ALA	A	43	-19.541	-0.360	19.306	1.00	34.77	AAAA
ATOM	273	CA	ALA	A	43	-19.920	-1.760	19.127	1.00	37.23	AAAA
ATOM	274	CB	ALA	A	43	-21.173	-2.060	19.948	1.00	37.66	AAAA
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ATOM	277	N	ASP	A	44	-20.333	-1.304	16.757	1.00	40.78	AAAA
ATOM	278	CA	ASP	A	44	-20.557	-1.671	15.361	1.00	42.78	AAAA
ATOM	279	CB	ASP	A	44	-21.678	-0.812	14.774	1.00	44.80	AAAA
ATOM	280	CG	ASP	A	44	-21.438	0.670	14.973	1.00	46.37	AAAA
ATOM	281	OD1	ASP	A	44	-20.464	1.206	14.400	1.00	48.22	AAAA
ATOM	282	OD2	ASP	A	44	-22.220	1.302	15.712	1.00	49.14	AAAA
ATOM	283	C	ASP	A	44	-19.324	-1.559	14.472	1.00	43.14	AAAA
ATOM	284	O	ASP	A	44	-19.320	-2.061	13.349	1.00	44.14	AAAA
ATOM	285	N	ARG	A	45	-18.281	-0.904	14.970	1.00	42.77	AAAA
ATOM	286	CA	ARG	A	45	-17.056	-0.730	14.199	1.00	42.34	AAAA
ATOM	287	CB	ARG	A	45	-16.415	0.614	14.550	1.00	44.43	AAAA
ATOM	288	CG	ARG	A	45	-17.206	1.822	14.056	1.00	48.23	AAAA
ATOM	289	CD	ARG	A	45	-17.272	1.845	12.533	1.00	51.20	AAAA

ATOM	290	NE	ARG	A	45	-17.950	3.029	12.014	1.00	54.35	AAAA
ATOM	291	CZ	ARG	A	45	-17.526	4.279	12.191	1.00	56.26	AAAA
ATOM	292	NH1	ARG	A	45	-16.417	4.522	12.881	1.00	56.45	AAAA
ATOM	293	NH2	ARG	A	45	-18.212	5.290	11.670	1.00	57.50	AAAA
ATOM	294	C	ARG	A	45	-16.054	-1.872	14.401	1.00	41.11	AAAA
ATOM	295	O	ARG	A	45	-16.194	-2.679	15.320	1.00	40.45	AAAA
ATOM	296	N	MET	A	46	-15.041	-1.928	13.543	1.00	39.55	AAAA
ATOM	297	CA	MET	A	46	-14.038	-2.990	13.604	1.00	39.67	AAAA
ATOM	298	CB	MET	A	46	-13.041	-2.839	12.444	1.00	39.68	AAAA
ATOM	299	CG	MET	A	46	-12.239	-1.544	12.423	1.00	42.15	AAAA
ATOM	300	SD	MET	A	46	-10.690	-1.620	13.352	1.00	44.74	AAAA
ATOM	301	CE	MET	A	46	-9.559	-2.332	12.128	1.00	41.92	AAAA
ATOM	302	C	MET	A	46	-13.279	-3.148	14.926	1.00	38.68	AAAA
ATOM	303	O	MET	A	46	-12.772	-4.232	15.219	1.00	38.02	AAAA
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ATOM	305	CA	GLU	A	47	-12.486	-2.198	17.002	1.00	36.91	AAAA
ATOM	306	CB	GLU	A	47	-12.309	-0.820	17.650	1.00	35.19	AAAA
ATOM	307	CG	GLU	A	47	-13.615	-0.150	18.058	1.00	34.12	AAAA
ATOM	308	CD	GLU	A	47	-14.142	0.807	17.003	1.00	34.06	AAAA
ATOM	309	OE1	GLU	A	47	-13.712	0.707	15.832	1.00	33.13	AAAA
ATOM	310	OE2	GLU	A	47	-14.995	1.652	17.350	1.00	32.08	AAAA
ATOM	311	C	GLU	A	47	-13.225	-3.123	17.972	1.00	36.96	AAAA
ATOM	312	O	GLU	A	47	-12.612	-3.744	18.842	1.00	37.00	AAAA
ATOM	313	N	ALA	A	48	-14.541	-3.222	17.818	1.00	36.76	AAAA
ATOM	314	CA	ALA	A	48	-15.342	-4.066	18.700	1.00	36.98	AAAA
ATOM	315	CB	ALA	A	48	-16.823	-3.917	18.365	1.00	37.33	AAAA
ATOM	316	C	ALA	A	48	-14.943	-5.533	18.623	1.00	38.23	AAAA
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ATOM	327	CA	LEU	A	50	-10.306	-6.623	16.982	1.00	39.05	AAAA
ATOM	328	CB	LEU	A	50	-9.710	-5.578	16.036	1.00	38.17	AAAA
ATOM	329	CG	LEU	A	50	-8.183	-5.562	15.942	1.00	38.18	AAAA
ATOM	330	CD1	LEU	A	50	-7.685	-6.916	15.462	1.00	37.91	AAAA
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ATOM	332	C	LEU	A	50	-9.666	-6.486	18.365	1.00	39.12	AAAA
ATOM	333	O	LEU	A	50	-8.805	-7.286	18.732	1.00	38.56	AAAA
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ATOM	337	CG1	VAL	A	51	-9.571	-3.795	22.523	1.00	35.15	AAAA
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ATOM	339	C	VAL	A	51	-9.647	-6.449	21.415	1.00	37.87	AAAA
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ATOM	349	CA	LYS	A	53	-8.752	-10.463	20.193	1.00	40.58	AAAA
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ATOM	353	CE	LYS	A	53	-11.280	-12.102	16.133	1.00	45.87	AAAA
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ATOM    356  O   LYS A  53      -6.426 -11.006  20.432  1.00 39.70 AAAA
ATOM    357  N   HIS A  54      -7.112  -9.014  21.231  1.00 38.65 AAAA
ATOM    358  CA  HIS A  54      -5.790  -8.642  21.727  1.00 37.71 AAAA
ATOM    359  CB  HIS A  54      -5.408  -7.233  21.272  1.00 37.50 AAAA
ATOM    360  CG  HIS A  54      -4.903  -7.164  19.864  1.00 37.59 AAAA
ATOM    361  CD2 HIS A  54      -5.483  -7.502  18.687  1.00 37.67 AAAA
ATOM    362  ND1 HIS A  54      -3.658  -6.666  19.546  1.00 37.90 AAAA
ATOM    363  CE1 HIS A  54      -3.492  -6.698  18.235  1.00 37.11 AAAA
ATOM    364  NE2 HIS A  54      -4.586  -7.202  17.691  1.00 36.75 AAAA
ATOM    365  C   HIS A  54      -5.788  -8.711  23.248  1.00 37.10 AAAA
ATOM    366  O   HIS A  54      -4.871  -8.214  23.899  1.00 37.35 AAAA
ATOM    367  N   GLY A  55      -6.828  -9.331  23.800  1.00 36.15 AAAA
ATOM    368  CA  GLY A  55      -6.948  -9.477  25.240  1.00 36.70 AAAA
ATOM    369  C   GLY A  55      -7.266  -8.200  25.997  1.00 36.66 AAAA
ATOM    370  O   GLY A  55      -7.145  -8.157  27.222  1.00 36.89 AAAA
ATOM    371  N   ILE A  56      -7.686  -7.163  25.277  1.00 35.61 AAAA
ATOM    372  CA  ILE A  56      -8.009  -5.885  25.900  1.00 34.03 AAAA
ATOM    373  CB  ILE A  56      -7.389  -4.723  25.100  1.00 32.39 AAAA
ATOM    374  CG2 ILE A  56      -7.748  -3.386  25.750  1.00 31.80 AAAA
ATOM    375  CG1 ILE A  56      -5.869  -4.904  25.031  1.00 31.50 AAAA
ATOM    376  CD1 ILE A  56      -5.149  -3.900  24.144  1.00 30.46 AAAA
ATOM    377  C   ILE A  56      -9.516  -5.668  26.017  1.00 34.37 AAAA
ATOM    378  O   ILE A  56     -10.263  -5.908  25.067  1.00 34.29 AAAA
ATOM    379  N   GLU A  57      -9.955  -5.224  27.193  1.00 34.18 AAAA
ATOM    380  CA  GLU A  57     -11.370  -4.969  27.432  1.00 34.19 AAAA
ATOM    381  CB  GLU A  57     -11.638  -4.733  28.922  1.00 37.08 AAAA
ATOM    382  CG  GLU A  57     -11.301  -5.913  29.837  1.00 41.06 AAAA
ATOM    383  CD  GLU A  57     -12.180  -7.127  29.591  1.00 44.07 AAAA
ATOM    384  OE1 GLU A  57     -12.011  -8.135  30.313  1.00 45.83 AAAA
ATOM    385  OE2 GLU A  57     -13.040  -7.078  28.682  1.00 46.00 AAAA
ATOM    386  C   GLU A  57     -11.751  -3.723  26.645  1.00 32.88 AAAA
ATOM    387  O   GLU A  57     -10.905  -2.870  26.368  1.00 31.69 AAAA
ATOM    388  N   ILE A  58     -13.022  -3.611  26.285  1.00 31.36 AAAA
ATOM    389  CA  ILE A  58     -13.454  -2.454  25.529  1.00 29.92 AAAA
ATOM    390  CB  ILE A  58     -13.390  -2.749  24.009  1.00 29.51 AAAA
ATOM    391  CG2 ILE A  58     -14.175  -4.015  23.689  1.00 28.67 AAAA
ATOM    392  CG1 ILE A  58     -13.895  -1.543  23.216  1.00 29.61 AAAA
ATOM    393  CD1 ILE A  58     -13.578  -1.623  21.734  1.00 29.09 AAAA
ATOM    394  C   ILE A  58     -14.843  -1.984  25.927  1.00 29.49 AAAA
ATOM    395  O   ILE A  58     -15.791  -2.764  25.968  1.00 27.83 AAAA
ATOM    396  N   ASP A  59     -14.939  -0.700  26.252  1.00 29.28 AAAA
ATOM    397  CA  ASP A  59     -16.202  -0.091  26.626  1.00 29.70 AAAA
ATOM    398  CB  ASP A  59     -15.999   0.916  27.759  1.00 30.90 AAAA
ATOM    399  CG  ASP A  59     -15.676   0.245  29.083  1.00 32.17 AAAA
ATOM    400  OD1 ASP A  59     -16.485  -0.591  29.540  1.00 33.00 AAAA
ATOM    401  OD2 ASP A  59     -14.615   0.554  29.664  1.00 33.03 AAAA
ATOM    402  C   ASP A  59     -16.723   0.608  25.378  1.00 30.39 AAAA
ATOM    403  O   ASP A  59     -15.947   1.165  24.600  1.00 30.45 AAAA
ATOM    404  N   PHE A  60     -18.033   0.570  25.180  1.00 31.29 AAAA
ATOM    405  CA  PHE A  60     -18.612   1.183  24.000  1.00 32.36 AAAA
ATOM    406  CB  PHE A  60     -19.469   0.166  23.239  1.00 33.01 AAAA
ATOM    407  CG  PHE A  60     -18.720  -1.056  22.793  1.00 33.55 AAAA
ATOM    408  CD1 PHE A  60     -19.033  -2.307  23.318  1.00 34.07 AAAA
ATOM    409  CD2 PHE A  60     -17.720  -0.964  21.832  1.00 34.02 AAAA
ATOM    410  CE1 PHE A  60     -18.362  -3.451  22.890  1.00 33.73 AAAA
ATOM    411  CE2 PHE A  60     -17.042  -2.104  21.397  1.00 34.93 AAAA
ATOM    412  CZ  PHE A  60     -17.366  -3.348  21.928  1.00 34.12 AAAA
ATOM    413  C   PHE A  60     -19.469   2.395  24.300  1.00 32.89 AAAA
ATOM    414  O   PHE A  60     -20.062   2.508  25.372  1.00 33.13 AAAA
ATOM    415  N   ILE A  61     -19.502   3.309  23.338  1.00 34.43 AAAA
ATOM    416  CA  ILE A  61     -20.326   4.500  23.421  1.00 36.08 AAAA
ATOM    417  CB  ILE A  61     -19.545   5.785  23.056  1.00 36.15 AAAA
ATOM    418  CG2 ILE A  61     -20.511   6.957  22.913  1.00 36.47 AAAA
ATOM    419  CG1 ILE A  61     -18.504   6.092  24.136  1.00 37.27 AAAA
ATOM    420  CD1 ILE A  61     -17.711   7.360  23.875  1.00 38.32 AAAA
ATOM    421  C   ILE A  61     -21.380   4.230  22.353  1.00 37.27 AAAA
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ATOM	422	O	ILE	A	61	-21.050	3.901	21.215	1.00	36.29 AAAA
ATOM	423	N	ARG	A	62	-22.644	4.337	22.728	1.00	39.91 AAAA
ATOM	424	CA	ARG	A	62	-23.732	4.087	21.797	1.00	43.16 AAAA
ATOM	425	CB	ARG	A	62	-24.818	3.268	22.494	1.00	44.19 AAAA
ATOM	426	CG	ARG	A	62	-26.183	3.312	21.825	1.00	48.33 AAAA
ATOM	427	CD	ARG	A	62	-27.207	2.581	22.680	1.00	50.28 AAAA
ATOM	428	NE	ARG	A	62	-28.584	2.906	22.319	1.00	52.71 AAAA
ATOM	429	CZ	ARG	A	62	-29.646	2.419	22.951	1.00	53.14 AAAA
ATOM	430	NH1	ARG	A	62	-29.482	1.586	23.968	1.00	54.03 AAAA
ATOM	431	NH2	ARG	A	62	-30.870	2.767	22.573	1.00	53.49 AAAA
ATOM	432	C	ARG	A	62	-24.302	5.400	21.280	1.00	44.33 AAAA
ATOM	433	O	ARG	A	62	-24.942	6.140	22.021	1.00	43.98 AAAA
ATOM	434	N	ILE	A	63	-24.053	5.686	20.005	1.00	46.60 AAAA
ATOM	435	CA	ILE	A	63	-24.537	6.912	19.378	1.00	49.26 AAAA
ATOM	436	CB	ILE	A	63	-23.369	7.834	18.965	1.00	49.17 AAAA
ATOM	437	CG2	ILE	A	63	-23.903	9.208	18.593	1.00	50.31 AAAA
ATOM	438	CG1	ILE	A	63	-22.368	7.967	20.113	1.00	49.48 AAAA
ATOM	439	CD1	ILE	A	63	-21.158	8.822	19.775	1.00	49.03 AAAA
ATOM	440	C	ILE	A	63	-25.316	6.540	18.123	1.00	50.72 AAAA
ATOM	441	O	ILE	A	63	-24.724	6.219	17.093	1.00	50.90 AAAA
ATOM	442	N	SER	A	64	-26.639	6.591	18.209	1.00	52.58 AAAA
ATOM	443	CA	SER	A	64	-27.488	6.235	17.078	1.00	54.45 AAAA
ATOM	444	CB	SER	A	64	-28.731	5.491	17.574	1.00	54.65 AAAA
ATOM	445	OG	SER	A	64	-29.528	6.329	18.391	1.00	55.29 AAAA
ATOM	446	C	SER	A	64	-27.927	7.433	16.242	1.00	55.33 AAAA
ATOM	447	O	SER	A	64	-27.919	8.571	16.713	1.00	55.34 AAAA
ATOM	448	N	GLY	A	65	-28.301	7.158	14.993	1.00	56.31 AAAA
ATOM	449	CA	GLY	A	65	-28.774	8.196	14.090	1.00	57.42 AAAA
ATOM	450	C	GLY	A	65	-27.751	9.156	13.508	1.00	58.34 AAAA
ATOM	451	O	GLY	A	65	-28.052	10.333	13.315	1.00	58.53 AAAA
ATOM	452	N	LEU	A	66	-26.552	8.668	13.207	1.00	59.08 AAAA
ATOM	453	CA	LEU	A	66	-25.514	9.530	12.648	1.00	59.80 AAAA
ATOM	454	CB	LEU	A	66	-24.147	9.153	13.229	1.00	59.99 AAAA
ATOM	455	CG	LEU	A	66	-23.927	9.513	14.704	1.00	60.38 AAAA
ATOM	456	CD1	LEU	A	66	-23.983	11.026	14.877	1.00	60.37 AAAA
ATOM	457	CD2	LEU	A	66	-24.983	8.840	15.565	1.00	60.47 AAAA
ATOM	458	C	LEU	A	66	-25.467	9.497	11.121	1.00	60.04 AAAA
ATOM	459	O	LEU	A	66	-25.049	10.466	10.484	1.00	59.29 AAAA
ATOM	460	N	ARG	A	67	-25.892	8.378	10.541	1.00	60.97 AAAA
ATOM	461	CA	ARG	A	67	-25.923	8.224	9.089	1.00	61.57 AAAA
ATOM	462	CB	ARG	A	67	-26.860	9.273	8.484	1.00	62.96 AAAA
ATOM	463	CG	ARG	A	67	-28.340	8.984	8.698	1.00	65.29 AAAA
ATOM	464	CD	ARG	A	67	-29.138	10.270	8.842	1.00	66.93 AAAA
ATOM	465	NE	ARG	A	67	-30.566	10.067	8.611	1.00	68.58 AAAA
ATOM	466	CZ	ARG	A	67	-31.514	10.924	8.980	1.00	69.56 AAAA
ATOM	467	NH1	ARG	A	67	-31.192	12.048	9.607	1.00	69.39 AAAA
ATOM	468	NH2	ARG	A	67	-32.788	10.665	8.709	1.00	69.97 AAAA
ATOM	469	C	ARG	A	67	-24.558	8.301	8.409	1.00	61.08 AAAA
ATOM	470	O	ARG	A	67	-24.474	8.448	7.191	1.00	61.57 AAAA
ATOM	471	N	GLY	A	68	-23.489	8.204	9.189	1.00	60.22 AAAA
ATOM	472	CA	GLY	A	68	-22.161	8.249	8.605	1.00	58.95 AAAA
ATOM	473	C	GLY	A	68	-21.531	9.627	8.541	1.00	58.19 AAAA
ATOM	474	O	GLY	A	68	-20.373	9.763	8.140	1.00	58.31 AAAA
ATOM	475	N	LYS	A	69	-22.282	10.655	8.921	1.00	57.03 AAAA
ATOM	476	CA	LYS	A	69	-21.746	12.009	8.904	1.00	55.91 AAAA
ATOM	477	CB	LYS	A	69	-22.812	13.015	9.349	1.00	56.90 AAAA
ATOM	478	CG	LYS	A	69	-23.827	13.368	8.264	1.00	57.91 AAAA
ATOM	479	CD	LYS	A	69	-23.167	14.147	7.133	1.00	58.56 AAAA
ATOM	480	CE	LYS	A	69	-24.163	14.517	6.044	1.00	59.37 AAAA
ATOM	481	NZ	LYS	A	69	-23.522	15.327	4.965	1.00	59.41 AAAA
ATOM	482	C	LYS	A	69	-20.527	12.078	9.818	1.00	54.19 AAAA
ATOM	483	O	LYS	A	69	-19.447	12.480	9.392	1.00	54.69 AAAA
ATOM	484	N	GLY	A	70	-20.697	11.676	11.072	1.00	51.77 AAAA
ATOM	485	CA	GLY	A	70	-19.575	11.692	11.991	1.00	48.95 AAAA
ATOM	486	C	GLY	A	70	-19.668	12.687	13.129	1.00	46.84 AAAA
ATOM	487	O	GLY	A	70	-20.754	12.975	13.629	1.00	46.29 AAAA

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ATOM    488  N   ILE A  71     -18.515  13.221  13.523  1.00 45.26 AAAA
ATOM    489  CA  ILE A  71     -18.415  14.174  14.623  1.00 43.82 AAAA
ATOM    490  CB  ILE A  71     -16.936  14.463  14.959  1.00 42.91 AAAA
ATOM    491  CG2 ILE A  71     -16.262  15.142  13.786  1.00 42.86 AAAA
ATOM    492  CG1 ILE A  71     -16.839  15.325  16.217  1.00 41.89 AAAA
ATOM    493  CD1 ILE A  71     -17.324  14.619  17.471  1.00 42.12 AAAA
ATOM    494  C   ILE A  71     -19.127  15.501  14.367  1.00 43.91 AAAA
ATOM    495  O   ILE A  71     -19.635  16.125  15.296  1.00 43.71 AAAA
ATOM    496  N   LYS A  72     -19.154  15.935  13.112  1.00 43.92 AAAA
ATOM    497  CA  LYS A  72     -19.815  17.188  12.757  1.00 43.85 AAAA
ATOM    498  CB  LYS A  72     -19.559  17.526  11.284  1.00 45.17 AAAA
ATOM    499  CG  LYS A  72     -20.140  16.517  10.297  1.00 46.64 AAAA
ATOM    500  CD  LYS A  72     -19.590  15.112  10.516  1.00 47.65 AAAA
ATOM    501  CE  LYS A  72     -18.070  15.074  10.388  1.00 47.12 AAAA
ATOM    502  NZ  LYS A  72     -17.533  13.692  10.506  1.00 46.69 AAAA
ATOM    503  C   LYS A  72     -21.318  17.073  13.003  1.00 42.82 AAAA
ATOM    504  O   LYS A  72     -21.969  18.035  13.414  1.00 43.31 AAAA
ATOM    505  N   ALA A  73     -21.862  15.889  12.752  1.00 41.38 AAAA
ATOM    506  CA  ALA A  73     -23.282  15.650  12.954  1.00 39.79 AAAA
ATOM    507  CB  ALA A  73     -23.700  14.379  12.238  1.00 39.55 AAAA
ATOM    508  C   ALA A  73     -23.575  15.524  14.438  1.00 39.28 AAAA
ATOM    509  O   ALA A  73     -24.509  16.132  14.959  1.00 37.60 AAAA
ATOM    510  N   LEU A  74     -22.760  14.725  15.116  1.00 38.96 AAAA
ATOM    511  CA  LEU A  74     -22.933  14.498  16.541  1.00 38.75 AAAA
ATOM    512  CB  LEU A  74     -21.817  13.575  17.055  1.00 39.47 AAAA
ATOM    513  CG  LEU A  74     -21.826  13.192  18.536  1.00 39.30 AAAA
ATOM    514  CD1 LEU A  74     -21.439  14.383  19.366  1.00 40.12 AAAA
ATOM    515  CD2 LEU A  74     -23.199  12.673  18.936  1.00 39.66 AAAA
ATOM    516  C   LEU A  74     -22.938  15.808  17.317  1.00 38.15 AAAA
ATOM    517  O   LEU A  74     -23.768  16.012  18.206  1.00 37.74 AAAA
ATOM    518  N   ILE A  75     -22.014  16.699  16.982  1.00 38.08 AAAA
ATOM    519  CA  ILE A  75     -21.923  17.975  17.678  1.00 39.02 AAAA
ATOM    520  CB  ILE A  75     -20.605  18.707  17.319  1.00 40.76 AAAA
ATOM    521  CG2 ILE A  75     -20.616  19.109  15.856  1.00 41.16 AAAA
ATOM    522  CG1 ILE A  75     -20.426  19.938  18.209  1.00 42.50 AAAA
ATOM    523  CD1 ILE A  75     -20.302  19.616  19.690  1.00 44.15 AAAA
ATOM    524  C   ILE A  75     -23.114  18.886  17.377  1.00 38.41 AAAA
ATOM    525  O   ILE A  75     -23.396  19.818  18.130  1.00 38.12 AAAA
ATOM    526  N   ALA A  76     -23.816  18.602  16.283  1.00 38.04 AAAA
ATOM    527  CA  ALA A  76     -24.971  19.399  15.878  1.00 37.19 AAAA
ATOM    528  CB  ALA A  76     -25.060  19.454  14.350  1.00 37.36 AAAA
ATOM    529  C   ALA A  76     -26.268  18.847  16.455  1.00 36.15 AAAA
ATOM    530  O   ALA A  76     -27.352  19.323  16.124  1.00 35.97 AAAA
ATOM    531  N   ALA A  77     -26.156  17.834  17.309  1.00 34.42 AAAA
ATOM    532  CA  ALA A  77     -27.326  17.225  17.935  1.00 33.14 AAAA
ATOM    533  CB  ALA A  77     -27.460  15.780  17.499  1.00 33.13 AAAA
ATOM    534  C   ALA A  77     -27.125  17.311  19.443  1.00 32.59 AAAA
ATOM    535  O   ALA A  77     -26.502  16.436  20.042  1.00 31.09 AAAA
ATOM    536  N   PRO A  78     -27.664  18.372  20.073  1.00 32.06 AAAA
ATOM    537  CD  PRO A  78     -28.619  19.290  19.423  1.00 31.98 AAAA
ATOM    538  CA  PRO A  78     -27.577  18.653  21.514  1.00 31.07 AAAA
ATOM    539  CB  PRO A  78     -28.671  19.701  21.727  1.00 32.32 AAAA
ATOM    540  CG  PRO A  78     -28.703  20.427  20.414  1.00 32.04 AAAA
ATOM    541  C   PRO A  78     -27.748  17.450  22.443  1.00 30.50 AAAA
ATOM    542  O   PRO A  78     -26.874  17.155  23.257  1.00 29.52 AAAA
ATOM    543  N   LEU A  79     -28.878  16.766  22.334  1.00 28.95 AAAA
ATOM    544  CA  LEU A  79     -29.130  15.619  23.194  1.00 29.33 AAAA
ATOM    545  CB  LEU A  79     -30.573  15.137  23.023  1.00 29.48 AAAA
ATOM    546  CG  LEU A  79     -31.644  16.154  23.435  1.00 30.82 AAAA
ATOM    547  CD1 LEU A  79     -33.025  15.542  23.234  1.00 31.23 AAAA
ATOM    548  CD2 LEU A  79     -31.450  16.558  24.901  1.00 30.46 AAAA
ATOM    549  C   LEU A  79     -28.160  14.465  22.950  1.00 28.58 AAAA
ATOM    550  O   LEU A  79     -27.745  13.795  23.898  1.00 27.00 AAAA
ATOM    551  N   ARG A  80     -27.794  14.240  21.689  1.00 27.70 AAAA
ATOM    552  CA  ARG A  80     -26.877  13.156  21.348  1.00 28.33 AAAA
ATOM    553  CB  ARG A  80     -26.813  12.941  19.836  1.00 30.44 AAAA
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ATOM    554  CG  ARG A  80     -28.037  12.294  19.222  1.00 36.59 AAAA
ATOM    555  CD  ARG A  80     -27.657  11.616  17.915  1.00 38.91 AAAA
ATOM    556  NE  ARG A  80     -28.821  11.189  17.151  1.00 43.51 AAAA
ATOM    557  CZ  ARG A  80     -29.537  11.991  16.370  1.00 44.36 AAAA
ATOM    558  NH1 ARG A  80     -29.207  13.270  16.244  1.00 45.19 AAAA
ATOM    559  NH2 ARG A  80     -30.589  11.513  15.721  1.00 45.91 AAAA
ATOM    560  C   ARG A  80     -25.464  13.384  21.871  1.00 27.39 AAAA
ATOM    561  O   ARG A  80     -24.835  12.455  22.392  1.00 26.07 AAAA
ATOM    562  N   ILE A  81     -24.950  14.603  21.719  1.00 26.19 AAAA
ATOM    563  CA  ILE A  81     -23.608  14.886  22.217  1.00 24.89 AAAA
ATOM    564  CB  ILE A  81     -23.081  16.269  21.702  1.00 25.72 AAAA
ATOM    565  CG2 ILE A  81     -24.069  17.373  22.021  1.00 26.90 AAAA
ATOM    566  CG1 ILE A  81     -21.722  16.584  22.332  1.00 25.98 AAAA
ATOM    567  CD1 ILE A  81     -20.696  15.474  22.169  1.00 26.39 AAAA
ATOM    568  C   ILE A  81     -23.609  14.832  23.752  1.00 24.30 AAAA
ATOM    569  O   ILE A  81     -22.669  14.315  24.365  1.00 22.57 AAAA
ATOM    570  N   PHE A  82     -24.672  15.344  24.367  1.00 22.71 AAAA
ATOM    571  CA  PHE A  82     -24.800  15.333  25.827  1.00 22.28 AAAA
ATOM    572  CB  PHE A  82     -26.099  16.029  26.236  1.00 21.54 AAAA
ATOM    573  CG  PHE A  82     -26.281  16.184  27.730  1.00 20.67 AAAA
ATOM    574  CD1 PHE A  82     -25.244  16.644  28.538  1.00 21.08 AAAA
ATOM    575  CD2 PHE A  82     -27.512  15.907  28.318  1.00 21.44 AAAA
ATOM    576  CE1 PHE A  82     -25.430  16.831  29.916  1.00 20.18 AAAA
ATOM    577  CE2 PHE A  82     -27.719  16.093  29.700  1.00 19.77 AAAA
ATOM    578  CZ  PHE A  82     -26.678  16.555  30.497  1.00 20.80 AAAA
ATOM    579  C   PHE A  82     -24.797  13.887  26.330  1.00 21.61 AAAA
ATOM    580  O   PHE A  82     -24.091  13.536  27.285  1.00 21.05 AAAA
ATOM    581  N   ASN A  83     -25.577  13.042  25.669  1.00 21.80 AAAA
ATOM    582  CA  ASN A  83     -25.648  11.640  26.045  1.00 22.62 AAAA
ATOM    583  CB  ASN A  83     -26.806  10.969  25.296  1.00 22.62 AAAA
ATOM    584  CG  ASN A  83     -26.921   9.495  25.612  1.00 25.00 AAAA
ATOM    585  OD1 ASN A  83     -26.227   8.677  25.031  1.00 26.80 AAAA
ATOM    586  ND2 ASN A  83     -27.791   9.153  26.548  1.00 28.27 AAAA
ATOM    587  C   ASN A  83     -24.324  10.888  25.805  1.00 21.61 AAAA
ATOM    588  O   ASN A  83     -23.903  10.080  26.639  1.00 22.04 AAAA
ATOM    589  N   ALA A  84     -23.658  11.150  24.686  1.00 19.98 AAAA
ATOM    590  CA  ALA A  84     -22.383  10.480  24.401  1.00 19.25 AAAA
ATOM    591  CB  ALA A  84     -21.912  10.817  22.981  1.00 20.79 AAAA
ATOM    592  C   ALA A  84     -21.318  10.906  25.424  1.00 19.48 AAAA
ATOM    593  O   ALA A  84     -20.509  10.095  25.880  1.00 18.26 AAAA
ATOM    594  N   TRP A  85     -21.322  12.188  25.769  1.00 17.57 AAAA
ATOM    595  CA  TRP A  85     -20.390  12.736  26.749  1.00 18.15 AAAA
ATOM    596  CB  TRP A  85     -20.561  14.260  26.781  1.00 17.16 AAAA
ATOM    597  CG  TRP A  85     -19.863  15.007  27.892  1.00 16.32 AAAA
ATOM    598  CD2 TRP A  85     -20.300  16.233  28.472  1.00 16.29 AAAA
ATOM    599  CE2 TRP A  85     -19.340  16.605  29.445  1.00 15.39 AAAA
ATOM    600  CE3 TRP A  85     -21.413  17.062  28.266  1.00 16.28 AAAA
ATOM    601  CD1 TRP A  85     -18.677  14.682  28.519  1.00 15.58 AAAA
ATOM    602  NE1 TRP A  85     -18.364  15.639  29.454  1.00 14.76 AAAA
ATOM    603  CZ2 TRP A  85     -19.458  17.762  30.204  1.00 14.50 AAAA
ATOM    604  CZ3 TRP A  85     -21.530  18.218  29.027  1.00 16.55 AAAA
ATOM    605  CH2 TRP A  85     -20.553  18.558  29.988  1.00 15.65 AAAA
ATOM    606  C   TRP A  85     -20.639  12.099  28.125  1.00 19.04 AAAA
ATOM    607  O   TRP A  85     -19.696  11.691  28.820  1.00 17.64 AAAA
ATOM    608  N   ARG A  86     -21.903  11.986  28.516  1.00 18.52 AAAA
ATOM    609  CA  ARG A  86     -22.216  11.375  29.803  1.00 19.34 AAAA
ATOM    610  CB  ARG A  86     -23.675  11.654  30.181  1.00 19.24 AAAA
ATOM    611  CG  ARG A  86     -23.892  13.104  30.660  1.00 18.36 AAAA
ATOM    612  CD  ARG A  86     -25.318  13.357  31.154  1.00 19.61 AAAA
ATOM    613  NE  ARG A  86     -26.303  13.245  30.072  1.00 19.64 AAAA
ATOM    614  CZ  ARG A  86     -27.021  12.156  29.807  1.00 21.06 AAAA
ATOM    615  NH1 ARG A  86     -26.880  11.063  30.548  1.00 19.09 AAAA
ATOM    616  NH2 ARG A  86     -27.879  12.156  28.787  1.00 18.59 AAAA
ATOM    627  O   GLN A  87     -19.846   6.687  29.576  1.00 18.93 AAAA
ATOM    628  N   ALA A  88     -19.471   8.479  28.255  1.00 20.24 AAAA
ATOM    629  CA  ALA A  88     -18.023   8.436  28.412  1.00 20.23 AAAA
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ATOM    630  CB  ALA A  88     -17.355   9.386  27.419  1.00 18.84 AAAA
ATOM    631  C   ALA A  88     -17.622   8.787  29.841  1.00 20.11 AAAA
ATOM    632  O   ALA A  88     -16.687   8.202  30.388  1.00 20.39 AAAA
ATOM    633  N   ARG A  89     -18.309   9.745  30.454  1.00 18.15 AAAA
ATOM    634  CA  ARG A  89     -17.985  10.091  31.836  1.00 19.16 AAAA
ATOM    635  CB  ARG A  89     -18.797  11.302  32.313  1.00 16.58 AAAA
ATOM    636  CG  ARG A  89     -18.225  12.657  31.896  1.00 17.41 AAAA
ATOM    637  CD  ARG A  89     -19.196  13.769  32.284  1.00 15.10 AAAA
ATOM    638  NE  ARG A  89     -19.437  13.835  33.729  1.00 16.60 AAAA
ATOM    639  CZ  ARG A  89     -18.675  14.506  34.587  1.00 16.76 AAAA
ATOM    640  NH1 ARG A  89     -17.609  15.173  34.157  1.00 16.02 AAAA
ATOM    641  NH2 ARG A  89     -18.990  14.531  35.877  1.00 15.64 AAAA
ATOM    642  C   ARG A  89     -18.258   8.902  32.764  1.00 19.91 AAAA
ATOM    643  O   ARG A  89     -17.469   8.618  33.674  1.00 18.92 AAAA
ATOM    644  N   ALA A  90     -19.371   8.213  32.544  1.00 21.12 AAAA
ATOM    645  CA  ALA A  90     -19.719   7.063  33.386  1.00 23.31 AAAA
ATOM    646  CB  ALA A  90     -21.080   6.502  32.976  1.00 24.02 AAAA
ATOM    647  C   ALA A  90     -18.640   5.990  33.257  1.00 24.57 AAAA
ATOM    648  O   ALA A  90     -18.236   5.367  34.243  1.00 24.35 AAAA
ATOM    649  N   ILE A  91     -18.173   5.790  32.031  1.00 24.03 AAAA
ATOM    650  CA  ILE A  91     -17.135   4.816  31.746  1.00 24.73 AAAA
ATOM    651  CB  ILE A  91     -16.922   4.699  30.209  1.00 25.99 AAAA
ATOM    652  CG2 ILE A  91     -15.547   4.086  29.890  1.00 25.27 AAAA
ATOM    653  CG1 ILE A  91     -18.061   3.875  29.601  1.00 25.74 AAAA
ATOM    654  CD1 ILE A  91     -18.123   3.931  28.085  1.00 25.37 AAAA
ATOM    655  C   ILE A  91     -15.823   5.196  32.436  1.00 25.69 AAAA
ATOM    656  O   ILE A  91     -15.133   4.339  32.991  1.00 25.17 AAAA
ATOM    657  N   MET A  92     -15.482   6.481  32.410  1.00 24.39 AAAA
ATOM    658  CA  MET A  92     -14.243   6.933  33.024  1.00 24.61 AAAA
ATOM    659  CB  MET A  92     -13.798   8.258  32.391  1.00 23.19 AAAA
ATOM    660  CG  MET A  92     -13.480   8.088  30.908  1.00 21.54 AAAA
ATOM    661  SD  MET A  92     -12.816   9.554  30.108  1.00 21.51 AAAA
ATOM    662  CE  MET A  92     -12.756   9.008  28.463  1.00 17.14 AAAA
ATOM    663  C   MET A  92     -14.325   7.041  34.545  1.00 24.72 AAAA
ATOM    664  O   MET A  92     -13.311   6.918  35.236  1.00 24.71 AAAA
ATOM    665  N   LYS A  93     -15.524   7.262  35.070  1.00 24.64 AAAA
ATOM    666  CA  LYS A  93     -15.700   7.337  36.517  1.00 26.89 AAAA
ATOM    667  CB  LYS A  93     -17.102   7.840  36.864  1.00 27.06 AAAA
ATOM    668  CG  LYS A  93     -17.269   9.345  36.831  1.00 26.10 AAAA
ATOM    669  CD  LYS A  93     -18.641   9.742  37.366  1.00 28.56 AAAA
ATOM    670  CE  LYS A  93     -18.762  11.251  37.483  1.00 28.03 AAAA
ATOM    671  NZ  LYS A  93     -20.068  11.663  38.060  1.00 29.77 AAAA
ATOM    672  C   LYS A  93     -15.495   5.938  37.119  1.00 28.19 AAAA
ATOM    673  O   LYS A  93     -14.994   5.792  38.238  1.00 28.43 AAAA
ATOM    674  N   ALA A  94     -15.880   4.912  36.367  1.00 29.30 AAAA
ATOM    675  CA  ALA A  94     -15.736   3.532  36.831  1.00 30.63 AAAA
ATOM    676  CB  ALA A  94     -16.750   2.635  36.131  1.00 30.03 AAAA
ATOM    677  C   ALA A  94     -14.325   2.981  36.622  1.00 30.40 AAAA
ATOM    678  O   ALA A  94     -13.778   2.322  37.507  1.00 30.67 AAAA
ATOM    679  N   TYR A  95     -13.735   3.255  35.462  1.00 29.39 AAAA
ATOM    680  CA  TYR A  95     -12.394   2.764  35.163  1.00 29.94 AAAA
ATOM    681  CB  TYR A  95     -12.189   2.685  33.648  1.00 29.85 AAAA
ATOM    682  CG  TYR A  95     -10.838   2.151  33.224  1.00 31.64 AAAA
ATOM    683  CD1 TYR A  95     -10.382   0.907  33.669  1.00 31.90 AAAA
ATOM    684  CE1 TYR A  95      -9.139   0.414  33.270  1.00 32.14 AAAA
ATOM    685  CD2 TYR A  95     -10.015   2.886  32.370  1.00 30.90 AAAA
ATOM    686  CE2 TYR A  95      -8.779   2.405  31.969  1.00 31.95 AAAA
ATOM    687  CZ  TYR A  95      -8.345   1.167  32.423  1.00 32.95 AAAA
ATOM    688  OH  TYR A  95      -7.120   0.687  32.019  1.00 33.09 AAAA
ATOM    689  C   TYR A  95     -11.312   3.633  35.791  1.00 29.90 AAAA
ATOM    690  O   TYR A  95     -10.253   3.137  36.190  1.00 28.99 AAAA
ATOM    691  N   LYS A  96     -11.584   4.930  35.871  1.00 28.94 AAAA
ATOM    692  CA  LYS A  96     -10.658   5.893  36.452  1.00 29.17 AAAA
ATOM    693  CB  LYS A  96     -10.543   5.658  37.966  1.00 32.14 AAAA
ATOM    694  CG  LYS A  96     -11.871   5.829  38.690  1.00 35.57 AAAA
ATOM    695  CD  LYS A  96     -11.784   5.541  40.183  1.00 38.37 AAAA
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ATOM    696  CE  LYS A  96     -13.158   5.718  40.828  1.00 39.96 AAAA
ATOM    697  NZ  LYS A  96     -13.170   5.428  42.295  1.00 42.96 AAAA
ATOM    698  C   LYS A  96      -9.274   5.884  35.817  1.00 27.78 AAAA
ATOM    699  O   LYS A  96      -8.281   5.608  36.482  1.00 28.12 AAAA
ATOM    700  N   PRO A  97      -9.187   6.185  34.509  1.00 26.15 AAAA
ATOM    701  CD  PRO A  97     -10.258   6.519  33.547  1.00 24.76 AAAA
ATOM    702  CA  PRO A  97      -7.867   6.191  33.868  1.00 24.70 AAAA
ATOM    703  CB  PRO A  97      -8.202   6.241  32.381  1.00 23.96 AAAA
ATOM    704  CG  PRO A  97      -9.477   7.078  32.362  1.00 24.55 AAAA
ATOM    705  C   PRO A  97      -7.060   7.408  34.320  1.00 24.77 AAAA
ATOM    706  O   PRO A  97      -7.628   8.438  34.684  1.00 23.93 AAAA
ATOM    707  N   ASP A  98      -5.737   7.288  34.314  1.00 24.94 AAAA
ATOM    708  CA  ASP A  98      -4.890   8.404  34.717  1.00 24.75 AAAA
ATOM    709  CB  ASP A  98      -3.554   7.891  35.261  1.00 26.69 AAAA
ATOM    710  CG  ASP A  98      -3.725   7.040  36.509  1.00 28.25 AAAA
ATOM    711  OD1 ASP A  98      -3.546   5.808  36.426  1.00 28.34 AAAA
ATOM    712  OD2 ASP A  98      -4.053   7.603  37.569  1.00 29.50 AAAA
ATOM    713  C   ASP A  98      -4.654   9.328  33.529  1.00 23.89 AAAA
ATOM    714  O   ASP A  98      -4.267  10.486  33.681  1.00 22.57 AAAA
ATOM    715  N   VAL A  99      -4.918   8.807  32.339  1.00 24.10 AAAA
ATOM    716  CA  VAL A  99      -4.740   9.569  31.111  1.00 23.85 AAAA
ATOM    717  CB  VAL A  99      -3.237   9.633  30.730  1.00 25.11 AAAA
ATOM    718  CG1 VAL A  99      -2.684   8.220  30.614  1.00 25.72 AAAA
ATOM    719  CG2 VAL A  99      -3.044  10.372  29.420  1.00 24.76 AAAA
ATOM    720  C   VAL A  99      -5.498   8.865  29.989  1.00 22.90 AAAA
ATOM    721  O   VAL A  99      -5.767   7.667  30.073  1.00 22.05 AAAA
ATOM    722  N   VAL A 100      -5.869   9.613  28.951  1.00 22.07 AAAA
ATOM    723  CA  VAL A 100      -6.544   9.008  27.808  1.00 21.38 AAAA
ATOM    724  CB  VAL A 100      -8.038   9.451  27.663  1.00 21.17 AAAA
ATOM    725  CG1 VAL A 100      -8.804   9.095  28.914  1.00 21.06 AAAA
ATOM    726  CG2 VAL A 100      -8.139  10.942  27.354  1.00 22.14 AAAA
ATOM    727  C   VAL A 100      -5.777   9.398  26.559  1.00 21.31 AAAA
ATOM    728  O   VAL A 100      -5.244  10.505  26.464  1.00 21.01 AAAA
ATOM    729  N   LEU A 101      -5.701   8.468  25.612  1.00 21.54 AAAA
ATOM    730  CA  LEU A 101      -4.994   8.697  24.362  1.00 22.01 AAAA
ATOM    731  CB  LEU A 101      -3.944   7.599  24.139  1.00 23.42 AAAA
ATOM    732  CG  LEU A 101      -2.691   7.856  23.288  1.00 25.21 AAAA
ATOM    733  CD1 LEU A 101      -2.230   6.515  22.696  1.00 25.87 AAAA
ATOM    734  CD2 LEU A 101      -2.930   8.854  22.187  1.00 26.43 AAAA
ATOM    735  C   LEU A 101      -6.006   8.644  23.222  1.00 21.51 AAAA
ATOM    736  O   LEU A 101      -6.667   7.625  23.029  1.00 21.94 AAAA
ATOM    737  N   GLY A 102      -6.127   9.742  22.484  1.00 21.18 AAAA
ATOM    738  CA  GLY A 102      -7.043   9.780  21.358  1.00 21.84 AAAA
ATOM    739  C   GLY A 102      -6.246   9.586  20.079  1.00 21.20 AAAA
ATOM    740  O   GLY A 102      -5.294  10.324  19.837  1.00 22.62 AAAA
ATOM    741  N   MET A 103      -6.627   8.599  19.270  1.00 21.18 AAAA
ATOM    742  CA  MET A 103      -5.933   8.312  18.015  1.00 22.83 AAAA
ATOM    743  CB  MET A 103      -5.715   6.805  17.865  1.00 23.16 AAAA
ATOM    744  CG  MET A 103      -4.978   6.140  19.030  1.00 24.31 AAAA
ATOM    745  SD  MET A 103      -3.333   6.804  19.308  1.00 27.62 AAAA
ATOM    746  CE  MET A 103      -2.455   6.156  17.873  1.00 26.43 AAAA
ATOM    747  C   MET A 103      -6.709   8.823  16.795  1.00 23.47 AAAA
ATOM    748  O   MET A 103      -6.351   8.532  15.653  1.00 23.75 AAAA
ATOM    749  N   GLY A 104      -7.767   9.590  17.043  1.00 25.38 AAAA
ATOM    750  CA  GLY A 104      -8.585  10.114  15.959  1.00 25.56 AAAA
ATOM    751  C   GLY A 104      -9.878   9.326  15.833  1.00 25.55 AAAA
ATOM    752  O   GLY A 104     -10.004   8.241  16.404  1.00 26.58 AAAA
ATOM    753  N   GLY A 105     -10.840   9.854  15.082  1.00 26.06 AAAA
ATOM    754  CA  GLY A 105     -12.107   9.159  14.930  1.00 26.21 AAAA
ATOM    755  C   GLY A 105     -13.140   9.819  15.823  1.00 26.96 AAAA
ATOM    756  O   GLY A 105     -12.810  10.258  16.926  1.00 25.49 AAAA
ATOM    757  N   TYR A 106     -14.393   9.863  15.376  1.00 27.65 AAAA
ATOM    758  CA  TYR A 106     -15.434  10.534  16.145  1.00 28.10 AAAA
ATOM    759  CB  TYR A 106     -16.759  10.556  15.362  1.00 31.05 AAAA
ATOM    760  CG  TYR A 106     -17.536   9.257  15.303  1.00 33.49 AAAA
ATOM    761  CD1 TYR A 106     -18.269   8.802  16.400  1.00 34.81 AAAA
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ATOM	762	CE1	TYR	A	106	-19.038	7.634	16.323	1.00	36.18 AAAA
ATOM	763	CD2	TYR	A	106	-17.581	8.509	14.123	1.00	35.64 AAAA
ATOM	764	CE2	TYR	A	106	-18.343	7.344	14.032	1.00	36.47 AAAA
ATOM	765	CZ	TYR	A	106	-19.069	6.912	15.133	1.00	37.27 AAAA
ATOM	766	OH	TYR	A	106	-19.829	5.766	15.027	1.00	38.99 AAAA
ATOM	767	C	TYR	A	106	-15.678	10.072	17.576	1.00	26.46 AAAA
ATOM	768	O	TYR	A	106	-15.976	10.897	18.430	1.00	26.55 AAAA
ATOM	769	N	VAL	A	107	-15.549	8.780	17.858	1.00	25.31 AAAA
ATOM	770	CA	VAL	A	107	-15.783	8.318	19.223	1.00	23.91 AAAA
ATOM	771	CB	VAL	A	107	-15.659	6.772	19.335	1.00	25.47 AAAA
ATOM	772	CG1	VAL	A	107	-14.224	6.327	19.076	1.00	26.57 AAAA
ATOM	773	CG2	VAL	A	107	-16.126	6.315	20.711	1.00	24.96 AAAA
ATOM	774	C	VAL	A	107	-14.836	8.993	20.223	1.00	23.22 AAAA
ATOM	775	O	VAL	A	107	-15.190	9.190	21.389	1.00	23.17 AAAA
ATOM	776	N	SER	A	108	-13.650	9.381	19.765	1.00	23.13 AAAA
ATOM	777	CA	SER	A	108	-12.676	10.029	20.643	1.00	23.40 AAAA
ATOM	778	CB	SER	A	108	-11.301	10.108	19.967	1.00	23.85 AAAA
ATOM	779	OG	SER	A	108	-11.292	11.038	18.899	1.00	25.04 AAAA
ATOM	780	C	SER	A	108	-13.121	11.430	21.044	1.00	23.03 AAAA
ATOM	781	O	SER	A	108	-12.592	12.009	21.993	1.00	22.32 AAAA
ATOM	782	N	GLY	A	109	-14.089	11.979	20.310	1.00	21.84 AAAA
ATOM	783	CA	GLY	A	109	-14.583	13.307	20.627	1.00	21.98 AAAA
ATOM	784	C	GLY	A	109	-15.297	13.342	21.972	1.00	20.30 AAAA
ATOM	785	O	GLY	A	109	-14.898	14.088	22.856	1.00	21.37 AAAA
ATOM	786	N	PRO	A	110	-16.369	12.557	22.155	1.00	20.07 AAAA
ATOM	787	CD	PRO	A	110	-16.992	11.637	21.191	1.00	20.80 AAAA
ATOM	788	CA	PRO	A	110	-17.085	12.550	23.436	1.00	19.58 AAAA
ATOM	789	CB	PRO	A	110	-18.232	11.569	23.199	1.00	20.85 AAAA
ATOM	790	CG	PRO	A	110	-18.398	11.548	21.702	1.00	22.43 AAAA
ATOM	791	C	PRO	A	110	-16.136	12.031	24.524	1.00	18.52 AAAA
ATOM	792	O	PRO	A	110	-16.184	12.462	25.675	1.00	19.12 AAAA
ATOM	793	N	GLY	A	111	-15.286	11.086	24.140	1.00	19.12 AAAA
ATOM	794	CA	GLY	A	111	-14.332	10.525	25.087	1.00	18.87 AAAA
ATOM	795	C	GLY	A	111	-13.402	11.601	25.612	1.00	17.97 AAAA
ATOM	796	O	GLY	A	111	-13.208	11.730	26.813	1.00	19.32 AAAA
ATOM	797	N	GLY	A	112	-12.822	12.380	24.704	1.00	18.62 AAAA
ATOM	798	CA	GLY	A	112	-11.925	13.451	25.105	1.00	17.38 AAAA
ATOM	799	C	GLY	A	112	-12.610	14.509	25.957	1.00	17.36 AAAA
ATOM	800	O	GLY	A	112	-12.035	14.997	26.936	1.00	16.49 AAAA
ATOM	801	N	LEU	A	113	-13.837	14.864	25.583	1.00	16.45 AAAA
ATOM	802	CA	LEU	A	113	-14.611	15.866	26.314	1.00	17.35 AAAA
ATOM	803	CB	LEU	A	113	-15.974	16.079	25.640	1.00	17.68 AAAA
ATOM	804	CG	LEU	A	113	-16.735	17.409	25.805	1.00	21.99 AAAA
ATOM	805	CD1	LEU	A	113	-18.205	17.154	25.511	1.00	20.80 AAAA
ATOM	806	CD2	LEU	A	113	-16.570	18.007	27.178	1.00	22.94 AAAA
ATOM	807	C	LEU	A	113	-14.836	15.329	27.725	1.00	16.05 AAAA
ATOM	808	O	LEU	A	113	-14.695	16.045	28.711	1.00	16.63 AAAA
ATOM	809	N	ALA	A	114	-15.199	14.056	27.801	1.00	16.59 AAAA
ATOM	810	CA	ALA	A	114	-15.442	13.416	29.087	1.00	15.95 AAAA
ATOM	811	CB	ALA	A	114	-15.859	11.963	28.868	1.00	17.72 AAAA
ATOM	812	C	ALA	A	114	-14.194	13.492	29.968	1.00	15.37 AAAA
ATOM	813	O	ALA	A	114	-14.260	13.952	31.105	1.00	15.94 AAAA
ATOM	814	N	ALA	A	115	-13.053	13.050	29.452	1.00	16.63 AAAA
ATOM	815	CA	ALA	A	115	-11.820	13.098	30.251	1.00	15.65 AAAA
ATOM	816	CB	ALA	A	115	-10.641	12.518	29.450	1.00	15.52 AAAA
ATOM	817	C	ALA	A	115	-11.506	14.530	30.693	1.00	16.10 AAAA
ATOM	818	O	ALA	A	115	-11.141	14.777	31.841	1.00	15.67 AAAA
ATOM	819	N	TRP	A	116	-11.650	15.480	29.778	1.00	16.71 AAAA
ATOM	820	CA	TRP	A	116	-11.380	16.873	30.100	1.00	17.31 AAAA
ATOM	821	CB	TRP	A	116	-11.542	17.723	28.835	1.00	18.91 AAAA
ATOM	822	CG	TRP	A	116	-11.172	19.155	29.003	1.00	21.69 AAAA
ATOM	823	CD2	TRP	A	116	-12.008	20.277	28.740	1.00	23.65 AAAA
ATOM	824	CE2	TRP	A	116	-11.262	21.438	29.048	1.00	25.14 AAAA
ATOM	825	CE3	TRP	A	116	-13.321	20.418	28.268	1.00	26.49 AAAA
ATOM	826	CD1	TRP	A	116	-9.979	19.658	29.447	1.00	23.00 AAAA
ATOM	827	NE1	TRP	A	116	-10.025	21.032	29.479	1.00	24.96 AAAA

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ATOM    828  CZ2 TRP A 116     -11.785  22.724  28.902  1.00 26.16 AAAA
ATOM    829  CZ3 TRP A 116     -13.842  21.702  28.122  1.00 26.44 AAAA
ATOM    830  CH2 TRP A 116     -13.072  22.834  28.439  1.00 25.35 AAAA
ATOM    831  C   TRP A 116     -12.292  17.377  31.233  1.00 16.50 AAAA
ATOM    832  O   TRP A 116     -11.835  18.080  32.137  1.00 16.03 AAAA
ATOM    833  N   SER A 117     -13.565  16.990  31.200  1.00 16.73 AAAA
ATOM    834  CA  SER A 117     -14.528  17.399  32.229  1.00 17.06 AAAA
ATOM    835  CB  SER A 117     -15.961  17.116  31.762  1.00 16.18 AAAA
ATOM    836  OG  SER A 117     -16.270  15.731  31.743  1.00 18.31 AAAA
ATOM    837  C   SER A 117     -14.289  16.720  33.586  1.00 18.05 AAAA
ATOM    838  O   SER A 117     -14.837  17.147  34.605  1.00 17.79 AAAA
ATOM    839  N   LEU A 118     -13.466  15.678  33.594  1.00 18.13 AAAA
ATOM    840  CA  LEU A 118     -13.146  14.950  34.827  1.00 19.26 AAAA
ATOM    841  CB  LEU A 118     -13.262  13.441  34.587  1.00 18.09 AAAA
ATOM    842  CG  LEU A 118     -14.686  12.932  34.353  1.00 20.04 AAAA
ATOM    843  CD1 LEU A 118     -14.659  11.484  33.869  1.00 20.30 AAAA
ATOM    844  CD2 LEU A 118     -15.480  13.064  35.646  1.00 20.40 AAAA
ATOM    845  C   LEU A 118     -11.736  15.283  35.305  1.00 20.78 AAAA
ATOM    846  O   LEU A 118     -11.267  14.763  36.321  1.00 20.64 AAAA
ATOM    847  N   GLY A 119     -11.057  16.152  34.566  1.00 21.27 AAAA
ATOM    848  CA  GLY A 119      -9.706  16.537  34.943  1.00 21.97 AAAA
ATOM    849  C   GLY A 119      -8.648  15.519  34.550  1.00 21.55 AAAA
ATOM    850  O   GLY A 119      -7.515  15.582  35.034  1.00 21.92 AAAA
ATOM    851  N   ILE A 120      -9.009  14.584  33.678  1.00 20.43 AAAA
ATOM    852  CA  ILE A 120      -8.082  13.548  33.214  1.00 21.09 AAAA
ATOM    853  CB  ILE A 120      -8.853  12.270  32.836  1.00 20.95 AAAA
ATOM    854  CG2 ILE A 120      -7.902  11.226  32.275  1.00 22.20 AAAA
ATOM    855  CG1 ILE A 120      -9.624  11.748  34.051  1.00 22.05 AAAA
ATOM    856  CD1 ILE A 120     -10.688  10.709  33.689  1.00 21.95 AAAA
ATOM    857  C   ILE A 120      -7.358  14.088  31.978  1.00 20.81 AAAA
ATOM    858  O   ILE A 120      -8.001  14.465  31.004  1.00 21.35 AAAA
ATOM    859  N   PRO A 121      -6.013  14.131  31.999  1.00 20.67 AAAA
ATOM    860  CD  PRO A 121      -5.052  13.722  33.040  1.00 20.88 AAAA
ATOM    861  CA  PRO A 121      -5.320  14.658  30.819  1.00 20.52 AAAA
ATOM    862  CB  PRO A 121      -3.842  14.649  31.237  1.00 21.37 AAAA
ATOM    863  CG  PRO A 121      -3.777  13.532  32.240  1.00 22.04 AAAA
ATOM    864  C   PRO A 121      -5.580  13.893  29.536  1.00 19.38 AAAA
ATOM    865  O   PRO A 121      -5.717  12.671  29.538  1.00 18.17 AAAA
ATOM    866  N   VAL A 122      -5.647  14.645  28.442  1.00 20.01 AAAA
ATOM    867  CA  VAL A 122      -5.903  14.102  27.120  1.00 19.76 AAAA
ATOM    868  CB  VAL A 122      -7.047  14.866  26.421  1.00 18.63 AAAA
ATOM    869  CG1 VAL A 122      -7.286  14.281  25.033  1.00 20.46 AAAA
ATOM    870  CG2 VAL A 122      -8.320  14.790  27.264  1.00 20.31 AAAA
ATOM    871  C   VAL A 122      -4.672  14.205  26.223  1.00 19.39 AAAA
ATOM    872  O   VAL A 122      -4.096  15.282  26.069  1.00 19.66 AAAA
ATOM    873  N   VAL A 123      -4.284  13.079  25.634  1.00 19.86 AAAA
ATOM    874  CA  VAL A 123      -3.134  13.029  24.734  1.00 20.22 AAAA
ATOM    875  CB  VAL A 123      -2.086  11.982  25.200  1.00 20.59 AAAA
ATOM    876  CG1 VAL A 123      -0.898  11.957  24.226  1.00 20.51 AAAA
ATOM    877  CG2 VAL A 123      -1.602  12.317  26.606  1.00 17.21 AAAA
ATOM    878  C   VAL A 123      -3.684  12.600  23.381  1.00 21.06 AAAA
ATOM    879  O   VAL A 123      -4.482  11.666  23.300  1.00 22.10 AAAA
ATOM    880  N   LEU A 124      -3.269  13.284  22.325  1.00 21.08 AAAA
ATOM    881  CA  LEU A 124      -3.746  12.952  20.989  1.00 21.68 AAAA
ATOM    882  CB  LEU A 124      -4.463  14.149  20.366  1.00 21.81 AAAA
ATOM    883  CG  LEU A 124      -5.629  14.805  21.105  1.00 21.93 AAAA
ATOM    884  CD1 LEU A 124      -6.133  15.980  20.268  1.00 22.15 AAAA
ATOM    885  CD2 LEU A 124      -6.737  13.787  21.337  1.00 21.49 AAAA
ATOM    886  C   LEU A 124      -2.628  12.558  20.038  1.00 21.67 AAAA
ATOM    887  O   LEU A 124      -1.493  13.011  20.170  1.00 22.39 AAAA
ATOM    888  N   HIS A 125      -2.964  11.713  19.075  1.00 22.63 AAAA
ATOM    889  CA  HIS A 125      -2.014  11.336  18.036  1.00 24.74 AAAA
ATOM    890  CB  HIS A 125      -1.429   9.939  18.244  1.00 24.62 AAAA
ATOM    891  CG  HIS A 125      -0.471   9.540  17.162  1.00 27.30 AAAA
ATOM    892  CD2 HIS A 125      -0.629   8.744  16.079  1.00 27.23 AAAA
ATOM    893  ND1 HIS A 125       0.806  10.057  17.072  1.00 29.96 AAAA
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ATOM    894  CE1 HIS A 125       1.391   9.597  15.979  1.00 27.40 AAAA
ATOM    895  NE2 HIS A 125       0.541   8.799  15.358  1.00 28.94 AAAA
ATOM    896  C   HIS A 125      -2.763  11.364  16.705  1.00 24.38 AAAA
ATOM    897  O   HIS A 125      -3.813  10.741  16.565  1.00 23.93 AAAA
ATOM    898  N   GLU A 126      -2.233  12.111  15.744  1.00 24.36 AAAA
ATOM    899  CA  GLU A 126      -2.836  12.199  14.420  1.00 26.31 AAAA
ATOM    900  CB  GLU A 126      -2.992  13.664  14.005  1.00 25.81 AAAA
ATOM    901  CG  GLU A 126      -3.465  13.861  12.567  1.00 26.62 AAAA
ATOM    902  CD  GLU A 126      -4.795  13.196  12.288  1.00 27.69 AAAA
ATOM    903  OE1 GLU A 126      -5.785  13.544  12.965  1.00 27.90 AAAA
ATOM    904  OE2 GLU A 126      -4.855  12.326  11.391  1.00 27.53 AAAA
ATOM    905  C   GLU A 126      -1.901  11.472  13.456  1.00 27.49 AAAA
ATOM    906  O   GLU A 126      -0.727  11.819  13.349  1.00 27.87 AAAA
ATOM    907  N   GLN A 127      -2.423  10.463  12.765  1.00 28.80 AAAA
ATOM    908  CA  GLN A 127      -1.617   9.682  11.834  1.00 30.09 AAAA
ATOM    909  CB  GLN A 127      -2.192   8.264  11.688  1.00 28.89 AAAA
ATOM    910  CG  GLN A 127      -2.184   7.421  12.958  1.00 28.94 AAAA
ATOM    911  CD  GLN A 127      -3.456   7.578  13.775  1.00 29.34 AAAA
ATOM    912  OE1 GLN A 127      -4.543   7.207  13.329  1.00 29.36 AAAA
ATOM    913  NE2 GLN A 127      -3.326   8.131  14.973  1.00 28.70 AAAA
ATOM    914  C   GLN A 127      -1.455  10.277  10.438  1.00 30.92 AAAA
ATOM    915  O   GLN A 127      -0.428  10.068   9.794  1.00 31.21 AAAA
ATOM    916  N   ASN A 128      -2.448  11.038   9.986  1.00 32.48 AAAA
ATOM    917  CA  ASN A 128      -2.434  11.596   8.634  1.00 33.12 AAAA
ATOM    918  CB  ASN A 128      -3.864  11.589   8.083  1.00 32.20 AAAA
ATOM    919  CG  ASN A 128      -4.606  10.312   8.424  1.00 33.05 AAAA
ATOM    920  OD1 ASN A 128      -5.296  10.236   9.445  1.00 33.34 AAAA
ATOM    921  ND2 ASN A 128      -4.454   9.292   7.584  1.00 31.22 AAAA
ATOM    922  C   ASN A 128      -1.809  12.971   8.394  1.00 33.60 AAAA
ATOM    923  O   ASN A 128      -1.571  13.744   9.327  1.00 34.03 AAAA
ATOM    924  N   GLY A 129      -1.550  13.256   7.117  1.00 33.69 AAAA
ATOM    925  CA  GLY A 129      -0.959  14.524   6.718  1.00 33.68 AAAA
ATOM    926  C   GLY A 129      -1.903  15.682   6.972  1.00 33.41 AAAA
ATOM    927  O   GLY A 129      -1.482  16.834   7.057  1.00 32.92 AAAA
ATOM    928  N   ILE A 130      -3.192  15.374   7.070  1.00 33.49 AAAA
ATOM    929  CA  ILE A 130      -4.205  16.383   7.361  1.00 33.06 AAAA
ATOM    930  CB  ILE A 130      -5.204  16.570   6.206  1.00 33.49 AAAA
ATOM    931  CG2 ILE A 130      -4.548  17.358   5.083  1.00 35.66 AAAA
ATOM    932  CG1 ILE A 130      -5.736  15.209   5.751  1.00 34.45 AAAA
ATOM    933  CD1 ILE A 130      -6.775  15.279   4.665  1.00 35.68 AAAA
ATOM    934  C   ILE A 130      -4.964  15.892   8.584  1.00 32.19 AAAA
ATOM    935  O   ILE A 130      -5.379  14.733   8.644  1.00 32.07 AAAA
ATOM    936  N   ALA A 131      -5.135  16.771   9.561  1.00 31.26 AAAA
ATOM    937  CA  ALA A 131      -5.832  16.404  10.788  1.00 30.63 AAAA
ATOM    938  CB  ALA A 131      -5.735  17.547  11.800  1.00 30.70 AAAA
ATOM    939  C   ALA A 131      -7.292  16.038  10.556  1.00 30.27 AAAA
ATOM    940  O   ALA A 131      -7.992  16.682   9.774  1.00 30.54 AAAA
ATOM    941  N   GLY A 132      -7.743  14.987  11.232  1.00 29.03 AAAA
ATOM    942  CA  GLY A 132      -9.131  14.587  11.119  1.00 27.98 AAAA
ATOM    943  C   GLY A 132      -9.902  15.678  11.837  1.00 26.80 AAAA
ATOM    944  O   GLY A 132      -9.326  16.387  12.660  1.00 25.68 AAAA
ATOM    945  N   LEU A 133     -11.188  15.827  11.543  1.00 26.51 AAAA
ATOM    946  CA  LEU A 133     -11.973  16.882  12.186  1.00 26.70 AAAA
ATOM    947  CB  LEU A 133     -13.363  16.967  11.538  1.00 28.16 AAAA
ATOM    948  CG  LEU A 133     -14.275  18.138  11.936  1.00 28.52 AAAA
ATOM    949  CD1 LEU A 133     -14.889  17.874  13.280  1.00 32.18 AAAA
ATOM    950  CD2 LEU A 133     -13.486  19.436  11.960  1.00 30.27 AAAA
ATOM    951  C   LEU A 133     -12.097  16.713  13.703  1.00 25.88 AAAA
ATOM    952  O   LEU A 133     -12.063  17.700  14.444  1.00 26.12 AAAA
ATOM    953  N   THR A 134     -12.240  15.475  14.169  1.00 24.18 AAAA
ATOM    954  CA  THR A 134     -12.353  15.230  15.608  1.00 23.78 AAAA
ATOM    955  CB  THR A 134     -12.605  13.729  15.922  1.00 23.18 AAAA
ATOM    956  OG1 THR A 134     -13.814  13.300  15.285  1.00 23.74 AAAA
ATOM    957  CG2 THR A 134     -12.751  13.511  17.433  1.00 23.66 AAAA
ATOM    958  C   THR A 134     -11.071  15.671  16.315  1.00 22.68 AAAA
ATOM    959  O   THR A 134     -11.116  16.368  17.328  1.00 21.38 AAAA
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ATOM    960  N   ASN A 135      -9.927  15.267  15.771  1.00 23.98 AAAA
ATOM    961  CA  ASN A 135      -8.636  15.623  16.358  1.00 24.64 AAAA
ATOM    962  CB  ASN A 135      -7.488  14.936  15.597  1.00 24.49 AAAA
ATOM    963  CG  ASN A 135      -7.020  13.638  16.264  1.00 25.25 AAAA
ATOM    964  OD1 ASN A 135      -6.267  12.856  15.668  1.00 25.70 AAAA
ATOM    965  ND2 ASN A 135      -7.445  13.415  17.504  1.00 22.51 AAAA
ATOM    966  C   ASN A 135      -8.421  17.135  16.349  1.00 25.19 AAAA
ATOM    967  O   ASN A 135      -7.890  17.702  17.301  1.00 24.79 AAAA
ATOM    968  N   LYS A 136      -8.839  17.792  15.274  1.00 26.78 AAAA
ATOM    969  CA  LYS A 136      -8.661  19.234  15.177  1.00 28.71 AAAA
ATOM    970  CB  LYS A 136      -9.165  19.743  13.828  1.00 30.84 AAAA
ATOM    971  CG  LYS A 136      -8.816  21.195  13.563  1.00 34.68 AAAA
ATOM    972  CD  LYS A 136      -9.206  21.596  12.148  1.00 36.19 AAAA
ATOM    973  CE  LYS A 136      -8.810  23.033  11.846  1.00 37.78 AAAA
ATOM    974  NZ  LYS A 136      -9.124  23.414  10.432  1.00 40.33 AAAA
ATOM    975  C   LYS A 136      -9.370  19.981  16.304  1.00 28.66 AAAA
ATOM    976  O   LYS A 136      -8.803  20.900  16.902  1.00 28.47 AAAA
ATOM    977  N   TRP A 137     -10.606  19.589  16.596  1.00 28.05 AAAA
ATOM    978  CA  TRP A 137     -11.363  20.243  17.656  1.00 28.85 AAAA
ATOM    979  CB  TRP A 137     -12.855  19.921  17.516  1.00 31.86 AAAA
ATOM    980  CG  TRP A 137     -13.485  20.502  16.282  1.00 34.71 AAAA
ATOM    981  CD2 TRP A 137     -14.788  20.206  15.755  1.00 36.70 AAAA
ATOM    982  CE2 TRP A 137     -14.982  21.036  14.630  1.00 37.21 AAAA
ATOM    983  CE3 TRP A 137     -15.811  19.321  16.130  1.00 38.46 AAAA
ATOM    984  CD1 TRP A 137     -12.959  21.466  15.471  1.00 36.22 AAAA
ATOM    985  NE1 TRP A 137     -13.851  21.794  14.480  1.00 36.96 AAAA
ATOM    986  CZ2 TRP A 137     -16.160  21.010  13.869  1.00 38.57 AAAA
ATOM    987  CZ3 TRP A 137     -16.986  19.295  15.373  1.00 39.12 AAAA
ATOM    988  CH2 TRP A 137     -17.148  20.136  14.255  1.00 39.31 AAAA
ATOM    989  C   TRP A 137     -10.868  19.803  19.029  1.00 28.01 AAAA
ATOM    990  O   TRP A 137     -10.763  20.605  19.955  1.00 27.04 AAAA
ATOM    991  N   LEU A 138     -10.548  18.520  19.143  1.00 27.31 AAAA
ATOM    992  CA  LEU A 138     -10.072  17.943  20.393  1.00 26.35 AAAA
ATOM    993  CB  LEU A 138      -9.879  16.444  20.174  1.00 27.79 AAAA
ATOM    994  CG  LEU A 138     -10.054  15.384  21.262  1.00 30.24 AAAA
ATOM    995  CD1 LEU A 138     -11.263  15.650  22.142  1.00 29.67 AAAA
ATOM    996  CD2 LEU A 138     -10.178  14.036  20.562  1.00 30.06 AAAA
ATOM    997  C   LEU A 138      -8.772  18.609  20.834  1.00 25.34 AAAA
ATOM    998  O   LEU A 138      -8.532  18.814  22.030  1.00 23.81 AAAA
ATOM    999  N   ALA A 139      -7.931  18.953  19.865  1.00 26.03 AAAA
ATOM   1000  CA  ALA A 139      -6.657  19.595  20.160  1.00 26.05 AAAA
ATOM   1001  CB  ALA A 139      -5.918  19.934  18.858  1.00 26.98 AAAA
ATOM   1002  C   ALA A 139      -6.847  20.858  21.002  1.00 26.86 AAAA
ATOM   1003  O   ALA A 139      -5.929  21.286  21.697  1.00 26.11 AAAA
ATOM   1004  N   LYS A 140      -8.044  21.439  20.952  1.00 26.32 AAAA
ATOM   1005  CA  LYS A 140      -8.329  22.649  21.716  1.00 26.90 AAAA
ATOM   1006  CB  LYS A 140      -9.644  23.276  21.238  1.00 29.14 AAAA
ATOM   1007  CG  LYS A 140      -9.665  23.595  19.749  1.00 31.62 AAAA
ATOM   1008  CD  LYS A 140      -8.523  24.513  19.364  1.00 35.02 AAAA
ATOM   1009  CE  LYS A 140      -8.811  25.975  19.704  1.00 37.44 AAAA
ATOM   1010  NZ  LYS A 140      -9.865  26.555  18.812  1.00 40.43 AAAA
ATOM   1011  C   LYS A 140      -8.395  22.414  23.230  1.00 25.59 AAAA
ATOM   1012  O   LYS A 140      -8.333  23.361  24.004  1.00 24.94 AAAA
ATOM   1013  N   ILE A 141      -8.526  21.159  23.649  1.00 24.13 AAAA
ATOM   1014  CA  ILE A 141      -8.587  20.844  25.075  1.00 23.31 AAAA
ATOM   1015  CB  ILE A 141      -9.971  20.270  25.477  1.00 22.85 AAAA
ATOM   1016  CG2 ILE A 141     -11.046  21.355  25.372  1.00 23.88 AAAA
ATOM   1017  CG1 ILE A 141     -10.313  19.071  24.595  1.00 23.34 AAAA
ATOM   1018  CD1 ILE A 141     -11.574  18.339  25.012  1.00 25.61 AAAA
ATOM   1019  C   ILE A 141      -7.524  19.822  25.482  1.00 23.06 AAAA
ATOM   1020  O   ILE A 141      -7.427  19.450  26.655  1.00 22.52 AAAA
ATOM   1021  N   ALA A 142      -6.724  19.375  24.520  1.00 21.80 AAAA
ATOM   1022  CA  ALA A 142      -5.695  18.379  24.803  1.00 21.97 AAAA
ATOM   1023  CB  ALA A 142      -5.231  17.739  23.495  1.00 20.41 AAAA
ATOM   1024  C   ALA A 142      -4.491  18.924  25.580  1.00 21.11 AAAA
ATOM   1025  O   ALA A 142      -4.132  20.094  25.465  1.00 22.76 AAAA
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ATOM   1026  N   THR A 143      -3.887  18.056  26.384  1.00 21.92 AAAA
ATOM   1027  CA  THR A 143      -2.707  18.391  27.178  1.00 22.64 AAAA
ATOM   1028  CB  THR A 143      -2.598  17.450  28.400  1.00 23.91 AAAA
ATOM   1029  OG1 THR A 143      -3.751  17.635  29.232  1.00 25.42 AAAA
ATOM   1030  CG2 THR A 143      -1.329  17.735  29.209  1.00 24.48 AAAA
ATOM   1031  C   THR A 143      -1.454  18.235  26.312  1.00 22.79 AAAA
ATOM   1032  O   THR A 143      -0.444  18.910  26.517  1.00 23.30 AAAA
ATOM   1033  N   LYS A 144      -1.525  17.341  25.335  1.00 23.20 AAAA
ATOM   1034  CA  LYS A 144      -0.398  17.106  24.440  1.00 25.09 AAAA
ATOM   1035  CB  LYS A 144       0.565  16.083  25.049  1.00 25.01 AAAA
ATOM   1036  CG  LYS A 144       1.706  15.658  24.129  1.00 28.28 AAAA
ATOM   1037  CD  LYS A 144       2.604  16.838  23.747  1.00 27.48 AAAA
ATOM   1038  CE  LYS A 144       3.818  16.373  22.946  1.00 29.11 AAAA
ATOM   1039  NZ  LYS A 144       4.722  17.507  22.587  1.00 28.97 AAAA
ATOM   1040  C   LYS A 144      -0.896  16.595  23.102  1.00 24.77 AAAA
ATOM   1041  O   LYS A 144      -1.688  15.660  23.039  1.00 24.45 AAAA
ATOM   1042  N   VAL A 145      -0.432  17.218  22.030  1.00 24.92 AAAA
ATOM   1043  CA  VAL A 145      -0.830  16.793  20.701  1.00 25.14 AAAA
ATOM   1044  CB  VAL A 145      -1.510  17.938  19.919  1.00 24.18 AAAA
ATOM   1045  CG1 VAL A 145      -2.023  17.418  18.591  1.00 24.71 AAAA
ATOM   1046  CG2 VAL A 145      -2.658  18.528  20.740  1.00 25.82 AAAA
ATOM   1047  C   VAL A 145       0.420  16.356  19.950  1.00 25.49 AAAA
ATOM   1048  O   VAL A 145       1.449  17.034  19.995  1.00 25.76 AAAA
ATOM   1049  N   MET A 146       0.324  15.208  19.289  1.00 26.18 AAAA
ATOM   1050  CA  MET A 146       1.421  14.654  18.503  1.00 26.41 AAAA
ATOM   1051  CB  MET A 146       2.000  13.396  19.172  1.00 26.85 AAAA
ATOM   1052  CG  MET A 146       2.826  13.653  20.430  1.00 25.85 AAAA
ATOM   1053  SD  MET A 146       3.306  12.116  21.269  1.00 28.45 AAAA
ATOM   1054  CE  MET A 146       1.827  11.741  22.217  1.00 26.47 AAAA
ATOM   1055  C   MET A 146       0.860  14.293  17.131  1.00 27.20 AAAA
ATOM   1056  O   MET A 146      -0.311  13.934  16.998  1.00 25.68 AAAA
ATOM   1057  N   GLN A 147       1.701  14.395  16.111  1.00 28.03 AAAA
ATOM   1058  CA  GLN A 147       1.294  14.091  14.748  1.00 28.39 AAAA
ATOM   1059  CB  GLN A 147       1.067  15.388  13.979  1.00 28.65 AAAA
ATOM   1060  CG  GLN A 147       2.203  16.371  14.142  1.00 30.13 AAAA
ATOM   1061  CD  GLN A 147       2.006  17.653  13.360  1.00 29.84 AAAA
ATOM   1062  OE1 GLN A 147       2.730  18.629  13.565  1.00 32.18 AAAA
ATOM   1063  NE2 GLN A 147       1.036  17.657  12.453  1.00 29.40 AAAA
ATOM   1064  C   GLN A 147       2.394  13.274  14.085  1.00 29.45 AAAA
ATOM   1065  O   GLN A 147       3.570  13.420  14.424  1.00 29.21 AAAA
ATOM   1066  N   ALA A 148       2.010  12.412  13.150  1.00 29.90 AAAA
ATOM   1067  CA  ALA A 148       2.975  11.563  12.461  1.00 31.39 AAAA
ATOM   1068  CB  ALA A 148       2.254  10.468  11.690  1.00 30.97 AAAA
ATOM   1069  C   ALA A 148       3.846  12.373  11.514  1.00 32.66 AAAA
ATOM   1070  O   ALA A 148       5.071  12.231  11.517  1.00 32.76 AAAA
ATOM   1071  N   PHE A 149       3.205  13.220  10.712  1.00 33.44 AAAA
ATOM   1072  CA  PHE A 149       3.903  14.059   9.744  1.00 35.09 AAAA
ATOM   1073  CB  PHE A 149       3.367  13.814   8.332  1.00 34.59 AAAA
ATOM   1074  CG  PHE A 149       3.200  12.367   7.985  1.00 35.35 AAAA
ATOM   1075  CD1 PHE A 149       1.935  11.789   7.958  1.00 34.17 AAAA
ATOM   1076  CD2 PHE A 149       4.304  11.579   7.685  1.00 34.88 AAAA
ATOM   1077  CE1 PHE A 149       1.771  10.448   7.637  1.00 34.20 AAAA
ATOM   1078  CE2 PHE A 149       4.148  10.236   7.364  1.00 36.09 AAAA
ATOM   1079  CZ  PHE A 149       2.878   9.670   7.340  1.00 35.09 AAAA
ATOM   1080  C   PHE A 149       3.719  15.536  10.056  1.00 36.17 AAAA
ATOM   1081  O   PHE A 149       2.697  15.939  10.606  1.00 37.06 AAAA
ATOM   1082  N   PRO A 150       4.709  16.370   9.704  1.00 37.23 AAAA
ATOM   1083  CD  PRO A 150       6.002  16.078   9.056  1.00 37.75 AAAA
ATOM   1084  CA  PRO A 150       4.569  17.803   9.975  1.00 38.03 AAAA
ATOM   1085  CB  PRO A 150       5.967  18.341   9.682  1.00 38.69 AAAA
ATOM   1086  CG  PRO A 150       6.432  17.448   8.569  1.00 38.52 AAAA
ATOM   1087  C   PRO A 150       3.510  18.369   9.028  1.00 38.18 AAAA
ATOM   1088  O   PRO A 150       3.355  17.878   7.912  1.00 38.42 AAAA
ATOM   1089  N   GLY A 151       2.763  19.374   9.475  1.00 38.74 AAAA
ATOM   1090  CA  GLY A 151       1.749  19.952   8.609  1.00 38.66 AAAA
ATOM   1091  C   GLY A 151       0.300  19.705   8.996  1.00 38.69 AAAA
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ATOM   1092  O   GLY A 151     -0.571  20.502   8.645  1.00 38.08 AAAA
ATOM   1093  N   ALA A 152      0.024  18.602   9.689  1.00 38.70 AAAA
ATOM   1094  CA  ALA A 152     -1.343  18.311  10.112  1.00 38.90 AAAA
ATOM   1095  CB  ALA A 152     -1.402  16.980  10.859  1.00 38.46 AAAA
ATOM   1096  C   ALA A 152     -1.729  19.461  11.032  1.00 39.30 AAAA
ATOM   1097  O   ALA A 152     -2.753  20.114  10.838  1.00 40.05 AAAA
ATOM   1098  N   PHE A 153     -0.887  19.700  12.031  1.00 39.42 AAAA
ATOM   1099  CA  PHE A 153     -1.084  20.795  12.971  1.00 39.90 AAAA
ATOM   1100  CB  PHE A 153     -1.209  20.286  14.409  1.00 39.04 AAAA
ATOM   1101  CG  PHE A 153     -2.478  19.535  14.685  1.00 38.06 AAAA
ATOM   1102  CD1 PHE A 153     -2.571  18.175  14.419  1.00 36.71 AAAA
ATOM   1103  CD2 PHE A 153     -3.582  20.190  15.228  1.00 37.52 AAAA
ATOM   1104  CE1 PHE A 153     -3.747  17.475  14.692  1.00 36.39 AAAA
ATOM   1105  CE2 PHE A 153     -4.761  19.500  15.502  1.00 36.08 AAAA
ATOM   1106  CZ  PHE A 153     -4.842  18.140  15.235  1.00 36.20 AAAA
ATOM   1107  C   PHE A 153      0.143  21.696  12.865  1.00 40.75 AAAA
ATOM   1108  O   PHE A 153      1.238  21.228  12.543  1.00 41.03 AAAA
ATOM   1109  N   PRO A 154     -0.026  23.001  13.128  1.00 41.05 AAAA
ATOM   1110  CD  PRO A 154     -1.328  23.667  13.304  1.00 41.17 AAAA
ATOM   1111  CA  PRO A 154      1.052  23.992  13.068  1.00 41.57 AAAA
ATOM   1112  CB  PRO A 154      0.339  25.292  13.428  1.00 41.69 AAAA
ATOM   1113  CG  PRO A 154     -1.024  25.081  12.876  1.00 41.76 AAAA
ATOM   1114  C   PRO A 154      2.260  23.744  13.975  1.00 42.12 AAAA
ATOM   1115  O   PRO A 154      3.400  23.833  13.515  1.00 43.15 AAAA
ATOM   1116  N   ASN A 155      2.023  23.432  15.249  1.00 41.75 AAAA
ATOM   1117  CA  ASN A 155      3.135  23.230  16.180  1.00 41.57 AAAA
ATOM   1118  CB  ASN A 155      3.180  24.389  17.179  1.00 44.02 AAAA
ATOM   1119  CG  ASN A 155      2.961  25.736  16.522  1.00 45.69 AAAA
ATOM   1120  OD1 ASN A 155      1.862  26.045  16.058  1.00 47.64 AAAA
ATOM   1121  ND2 ASN A 155      4.010  26.545  16.475  1.00 47.43 AAAA
ATOM   1122  C   ASN A 155      3.193  21.921  16.970  1.00 40.83 AAAA
ATOM   1123  O   ASN A 155      3.973  21.814  17.917  1.00 41.17 AAAA
ATOM   1124  N   ALA A 156      2.390  20.929  16.601  1.00 38.83 AAAA
ATOM   1125  CA  ALA A 156      2.400  19.658  17.326  1.00 37.19 AAAA
ATOM   1126  CB  ALA A 156      1.203  18.811  16.909  1.00 36.03 AAAA
ATOM   1127  C   ALA A 156      3.698  18.882  17.090  1.00 35.95 AAAA
ATOM   1128  O   ALA A 156      4.206  18.834  15.971  1.00 35.55 AAAA
ATOM   1129  N   GLU A 157      4.233  18.275  18.146  1.00 35.08 AAAA
ATOM   1130  CA  GLU A 157      5.464  17.505  18.022  1.00 33.77 AAAA
ATOM   1131  CB  GLU A 157      5.848  16.881  19.373  1.00 34.33 AAAA
ATOM   1132  CG  GLU A 157      7.175  16.124  19.352  1.00 34.59 AAAA
ATOM   1133  CD  GLU A 157      7.487  15.430  20.670  1.00 35.45 AAAA
ATOM   1134  OE1 GLU A 157      8.517  14.729  20.746  1.00 34.09 AAAA
ATOM   1135  OE2 GLU A 157      6.705  15.582  21.631  1.00 36.21 AAAA
ATOM   1136  C   GLU A 157      5.282  16.405  16.970  1.00 32.70 AAAA
ATOM   1137  O   GLU A 157      4.262  15.709  16.952  1.00 31.88 AAAA
ATOM   1138  N   VAL A 158      6.268  16.265  16.088  1.00 31.00 AAAA
ATOM   1139  CA  VAL A 158      6.230  15.255  15.032  1.00 30.25 AAAA
ATOM   1140  CB  VAL A 158      6.926  15.768  13.751  1.00 30.33 AAAA
ATOM   1141  CG1 VAL A 158      7.013  14.653  12.719  1.00 29.98 AAAA
ATOM   1142  CG2 VAL A 158      6.147  16.953  13.181  1.00 30.15 AAAA
ATOM   1143  C   VAL A 158      6.937  13.998  15.529  1.00 29.69 AAAA
ATOM   1144  O   VAL A 158      8.142  14.020  15.798  1.00 29.80 AAAA
ATOM   1145  N   VAL A 159      6.182  12.909  15.645  1.00 28.61 AAAA
ATOM   1146  CA  VAL A 159      6.715  11.647  16.149  1.00 29.00 AAAA
ATOM   1147  CB  VAL A 159      6.019  11.250  17.469  1.00 28.75 AAAA
ATOM   1148  CG1 VAL A 159      6.129  12.384  18.482  1.00 28.06 AAAA
ATOM   1149  CG2 VAL A 159      4.552  10.921  17.197  1.00 28.06 AAAA
ATOM   1150  C   VAL A 159      6.581  10.469  15.186  1.00 29.32 AAAA
ATOM   1151  O   VAL A 159      7.066   9.376  15.479  1.00 29.89 AAAA
ATOM   1152  N   GLY A 160      5.915  10.688  14.054  1.00 30.03 AAAA
ATOM   1153  CA  GLY A 160      5.727   9.628  13.075  1.00 29.63 AAAA
ATOM   1154  C   GLY A 160      4.678   8.608  13.483  1.00 29.61 AAAA
ATOM   1155  O   GLY A 160      3.917   8.849  14.416  1.00 29.30 AAAA
ATOM   1156  N   ASN A 161      4.635   7.475  12.782  1.00 29.30 AAAA
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ATOM   1160  OD1 ASN A 161       0.951   7.461  12.492  1.00 31.78 AAAA
ATOM   1161  ND2 ASN A 161       1.750   7.711  10.400  1.00 30.88 AAAA
ATOM   1162  C   ASN A 161       4.344   5.089  13.462  1.00 29.50 AAAA
ATOM   1163  O   ASN A 161       5.471   4.810  13.058  1.00 29.61 AAAA
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ATOM   1165  CD  PRO A 162       2.441   4.571  15.039  1.00 29.95 AAAA
ATOM   1166  CA  PRO A 162       4.219   2.977  14.650  1.00 29.65 AAAA
ATOM   1167  CB  PRO A 162       3.143   2.389  15.553  1.00 29.79 AAAA
ATOM   1168  CG  PRO A 162       2.559   3.608  16.200  1.00 30.38 AAAA
ATOM   1169  C   PRO A 162       4.423   2.135  13.389  1.00 30.13 AAAA
ATOM   1170  O   PRO A 162       3.535   2.063  12.531  1.00 28.48 AAAA
ATOM   1171  N   VAL A 163       5.590   1.508  13.287  1.00 29.92 AAAA
ATOM   1172  CA  VAL A 163       5.935   0.664  12.149  1.00 29.89 AAAA
ATOM   1173  CB  VAL A 163       7.182   1.224  11.417  1.00 31.04 AAAA
ATOM   1174  CG1 VAL A 163       7.571   0.308  10.260  1.00 30.44 AAAA
ATOM   1175  CG2 VAL A 163       6.902   2.631  10.914  1.00 29.10 AAAA
ATOM   1176  C   VAL A 163       6.258  -0.744  12.652  1.00 31.06 AAAA
ATOM   1177  O   VAL A 163       6.884  -0.892  13.706  1.00 29.66 AAAA
ATOM   1178  N   ARG A 164       5.820  -1.773  11.927  1.00 31.83 AAAA
ATOM   1179  CA  ARG A 164       6.124  -3.142  12.339  1.00 34.34 AAAA
ATOM   1180  CB  ARG A 164       5.533  -4.167  11.354  1.00 36.31 AAAA
ATOM   1181  CG  ARG A 164       5.704  -3.841   9.876  1.00 39.86 AAAA
ATOM   1182  CD  ARG A 164       4.855  -4.770   8.997  1.00 41.13 AAAA
ATOM   1183  NE  ARG A 164       5.368  -6.140   8.946  1.00 43.44 AAAA
ATOM   1184  CZ  ARG A 164       4.765  -7.145   8.311  1.00 44.08 AAAA
ATOM   1185  NH1 ARG A 164       3.619  -6.940   7.671  1.00 44.91 AAAA
ATOM   1186  NH2 ARG A 164       5.308  -8.355   8.308  1.00 44.44 AAAA
ATOM   1187  C   ARG A 164       7.649  -3.248  12.419  1.00 34.72 AAAA
ATOM   1188  O   ARG A 164       8.364  -2.769  11.537  1.00 33.63 AAAA
ATOM   1189  N   THR A 165       8.138  -3.855  13.496  1.00 34.72 AAAA
ATOM   1190  CA  THR A 165       9.567  -3.969  13.730  1.00 34.94 AAAA
ATOM   1191  CB  THR A 165       9.839  -4.437  15.177  1.00 35.90 AAAA
ATOM   1192  OG1 THR A 165       9.008  -5.563  15.488  1.00 36.96 AAAA
ATOM   1193  CG2 THR A 165       9.530  -3.313  16.149  1.00 35.88 AAAA
ATOM   1194  C   THR A 165      10.373  -4.814  12.749  1.00 34.61 AAAA
ATOM   1195  O   THR A 165      11.577  -4.603  12.608  1.00 34.56 AAAA
ATOM   1196  N   ASP A 166       9.739  -5.765  12.068  1.00 34.66 AAAA
ATOM   1197  CA  ASP A 166      10.492  -6.558  11.103  1.00 34.85 AAAA
ATOM   1198  CB  ASP A 166       9.697  -7.784  10.642  1.00 36.47 AAAA
ATOM   1199  CG  ASP A 166       8.341  -7.430  10.089  1.00 37.65 AAAA
ATOM   1200  OD1 ASP A 166       7.566  -8.365   9.804  1.00 41.03 AAAA
ATOM   1201  OD2 ASP A 166       8.048  -6.227   9.937  1.00 39.97 AAAA
ATOM   1202  C   ASP A 166      10.862  -5.667   9.917  1.00 33.70 AAAA
ATOM   1203  O   ASP A 166      11.846  -5.925   9.224  1.00 34.04 AAAA
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ATOM   1206  CB  VAL A 167       9.096  -2.888   8.170  1.00 31.53
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ATOM   1208  CG2 VAL A 167       8.120  -3.825   7.458  1.00 31.61
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ATOM   1213  CB  LEU A 168      11.714  -0.942  12.387  1.00 33.77
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ATOM   1255  CA  GLN A 174      23.063   1.401   0.591  1.00 43.56
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ATOM AAAA	1398	NE2	GLN	A	193	-10.162	-7.853	2.567	1.00 45.80
ATOM AAAA	1399	C	GLN	A	193	-8.298	-6.098	-1.781	1.00 39.31
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ATOM 1714 CD GLN A 236 6.454 -9.088 -20.647 1.00 26.71 AAAA
ATOM 1715 OE1 GLN A 236 7.410 -9.488 -19.976 1.00 24.90 AAAA
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ATOM 1722 CB PRO A 237 2.998 -15.626 -18.531 1.00 22.52 AAAA
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AAAAATOM	2363	CB	TRP	A	322	13.008	5.688	-11.611	1.00 39.41
AAAAATOM	2364	CG	TRP	A	322	12.047	6.748	-11.146	1.00 40.01
AAAAATOM	2365	CD2	TRP	A	322	10.898	6.558	-10.307	1.00 40.49
AAAAATOM	2366	CE2	TRP	A	322	10.330	7.833	-10.081	1.00 41.27
AAAAATOM	2367	CE3	TRP	A	322	10.295	5.436	-9.722	1.00 40.54
AAAAATOM	2368	CD1	TRP	A	322	12.126	8.091	-11.389	1.00 39.97
AAAAATOM	2369	NE1	TRP	A	322	11.098	8.749	-10.752	1.00 40.69
AAAAATOM	2370	CZ2	TRP	A	322	9.186	8.018	-9.293	1.00 41.67
AAAAATOM	2371	CZ3	TRP	A	322	9.155	5.619	-8.938	1.00 41.40
AAAAATOM	2372	CH2	TRP	A	322	8.615	6.903	-8.732	1.00 41.69
AAAAATOM	2373	C	TRP	A	322	14.984	5.109	-13.027	1.00 38.48
AAAAATOM	2374	O	TRP	A	322	14.743	3.929	-13.271	1.00 38.22
AAAAATOM	2375	N	SER	A	323	16.217	5.596	-12.935	1.00 38.13
AAAAATOM	2376	CA	SER	A	323	17.395	4.753	-13.101	1.00 38.51
AAAAATOM	2377	CB	SER	A	323	18.573	5.590	-13.591	1.00 38.51
AAAAATOM	2378	OG	SER	A	323	18.994	6.489	-12.582	1.00 39.52
AAAAATOM	2379	C	SER	A	323	17.739	4.150	-11.744	1.00 38.37
AAAAATOM	2380	O	SER	A	323	17.188	4.566	-10.725	1.00 37.29
AAAAATOM	2381	N	ARG	A	324	18.647	3.178	-11.723	1.00 37.86
AAAAATOM	2382	CA	ARG	A	324	19.030	2.563	-10.461	1.00 37.82
AAAAATOM	2383	CB	ARG	A	324	19.924	1.341	-10.688	1.00 36.36
AAAAATOM	2384	CG	ARG	A	324	19.130	0.077	-10.959	1.00 34.77
AAAAATOM	2385	CD	ARG	A	324	19.978	-1.176	-10.849	1.00 33.04
AAAAATOM	2386	NE	ARG	A	324	19.143	-2.372	-10.888	1.00 31.23
AAAAATOM	2387	CZ	ARG	A	324	18.318	-2.738	-9.908	1.00 29.95
AAAAATOM	2388	NH1	ARG	A	324	18.228	-2.006	-8.808	1.00 28.46
AAAAATOM	2389	NH2	ARG	A	324	17.562	-3.815	-10.041	1.00 28.17
AAAAATOM	2390	C	ARG	A	324	19.731	3.571	-9.569	1.00 38.78
AAAAATOM	2391	O	ARG	A	324	19.532	3.578	-8.354	1.00 38.12
AAAAATOM	2392	N	GLU	A	325	20.551	4.428	-10.169	1.00 39.55
AAAAATOM	2393	CA	GLU	A	325	21.251	5.447	-9.401	1.00 40.60
AAAAATOM	2394	CB	GLU	A	325	22.208	6.236	-10.304	1.00 42.74
AAAAATOM	2395	CG	GLU	A	325	22.642	7.589	-9.745	1.00 46.19
AAAAATOM	2396	CD	GLU	A	325	23.197	7.517	-8.327	1.00 48.10
AAAAATOM	2397	OE1	GLU	A	325	23.535	8.586	-7.770	1.00 49.61
AAAAATOM	2398	OE2	GLU	A	325	23.297	6.403	-7.768	1.00 49.87
AAAAATOM	2399	C	GLU	A	325	20.214	6.380	-8.784	1.00 39.88
AAAAATOM	2400	O	GLU	A	325	20.324	6.771	-7.623	1.00 39.45
AAAAATOM	2401	N	THR	A	326	19.202	6.725	-9.572	1.00 39.89
AAAAATOM	2402	CA	THR	A	326	18.130	7.591	-9.102	1.00 40.25
AAAAATOM	2403	CB	THR	A	326	17.139	7.912	-10.240	1.00 40.72
AAAAATOM	2404	OG1	THR	A	326	17.828	8.593	-11.298	1.00 42.28
AAAAATOM	2405	CG2	THR	A	326	16.006	8.795	-9.730	1.00 41.64
AAAAATOM	2406	C	THR	A	326	17.371	6.897	-7.968	1.00 39.76
AAAAATOM	2407	O	THR	A	326	17.108	7.497	-6.925	1.00 39.87
AAAAATOM	2408	N	LEU	A	327	17.027	5.628	-8.175	1.00 38.46
AAAAATOM	2409	CA	LEU	A	327	16.294	4.867	-7.169	1.00 37.41
AAAAATOM	2410	CB	LEU	A	327	15.968	3.466	-7.697	1.00 36.19
AAAAATOM	2411	CG	LEU	A	327	14.952	3.426	-8.843	1.00 35.32
AAAAATOM	2412	CD1	LEU	A	327	14.802	2.002	-9.370	1.00 35.07
AAAAATOM	2413	CD2	LEU	A	327	13.614	3.961	-8.354	1.00 34.69
AAAAATOM	2414	C	LEU	A	327	17.050	4.774	-5.845	1.00 37.39
AAAAATOM	2415	O	LEU	A	327	16.437	4.807	-4.778	1.00 36.80
AAAAATOM	2416	N	LEU	A	328	18.375	4.665	-5.909	1.00 37.58
AAAAATOM	2417	CA	LEU	A	328	19.184	4.593	-4.693	1.00 38.35

AAAAATOM	2418	CB	LEU	A	328	20.662	4.368	-5.030	1.00	38.95
AAAAATOM	2419	CG	LEU	A	328	21.636	4.544	-3.854	1.00	40.10
AAAAATOM	2420	CD1	LEU	A	328	21.303	3.551	-2.752	1.00	39.51
AAAAATOM	2421	CD2	LEU	A	328	23.068	4.349	-4.330	1.00	40.30
AAAAATOM	2422	C	LEU	A	328	19.039	5.899	-3.926	1.00	38.68
AAAAATOM	2423	O	LEU	A	328	18.929	5.906	-2.697	1.00	38.65
AAAAATOM	2424	N	THR	A	329	19.048	7.004	-4.664	1.00	39.35
AAAAATOM	2425	CA	THR	A	329	18.908	8.326	-4.068	1.00	39.98
AAAAATOM	2426	CB	THR	A	329	19.002	9.433	-5.136	1.00	40.05
AAAAATOM	2427	OG1	THR	A	329	20.280	9.364	-5.782	1.00	41.54
AAAAATOM	2428	CG2	THR	A	329	18.841	10.808	-4.497	1.00	40.35
AAAAATOM	2429	C	THR	A	329	17.557	8.425	-3.367	1.00	39.68
AAAAATOM	2430	O	THR	A	329	17.485	8.743	-2.179	1.00	39.91
AAAAATOM	2431	N	MET	A	330	16.492	8.147	-4.111	1.00	39.51
AAAAATOM	2432	CA	MET	A	330	15.143	8.190	-3.564	1.00	38.79
AAAAATOM	2433	CB	MET	A	330	14.141	7.718	-4.617	1.00	38.09
AAAAATOM	2434	CG	MET	A	330	14.011	8.657	-5.804	1.00	36.84
AAAAATOM	2435	SD	MET	A	330	12.977	7.980	-7.108	1.00	37.95
AAAAATOM	2436	CE	MET	A	330	11.332	8.342	-6.478	1.00	37.58
AAAAATOM	2437	C	MET	A	330	15.037	7.315	-2.319	1.00	39.71
AAAAATOM	2438	O	MET	A	330	14.418	7.703	-1.326	1.00	39.60
AAAAATOM	2439	N	ALA	A	331	15.646	6.135	-2.381	1.00	39.50
AAAAATOM	2440	CA	ALA	A	331	15.625	5.202	-1.266	1.00	40.36
AAAAATOM	2441	CB	ALA	A	331	16.378	3.928	-1.634	1.00	39.91
AAAAATOM	2442	C	ALA	A	331	16.243	5.843	-0.032	1.00	40.98
AAAAATOM	2443	O	ALA	A	331	15.662	5.805	1.052	1.00	40.34
AAAAATOM	2444	N	GLU	A	332	17.422	6.435	-0.201	1.00	41.85
AAAAATOM	2445	CA	GLU	A	332	18.102	7.087	0.911	1.00	42.77
AAAAATOM	2446	CB	GLU	A	332	19.470	7.607	0.465	1.00	44.04
AAAAATOM	2447	CG	GLU	A	332	20.414	6.500	0.016	1.00	46.55
AAAAATOM	2448	CD	GLU	A	332	21.822	6.994	-0.248	1.00	48.04
AAAAATOM	2449	OE1	GLU	A	332	21.981	7.923	-1.065	1.00	49.87
AAAAATOM	2450	OE2	GLU	A	332	22.770	6.449	0.359	1.00	49.38
AAAAATOM	2451	C	GLU	A	332	17.246	8.228	1.445	1.00	42.38
AAAAATOM	2452	O	GLU	A	332	17.156	8.435	2.653	1.00	42.66
AAAAATOM	2453	N	ARG	A	333	16.619	8.969	0.540	1.00	41.80
AAAAATOM	2454	CA	ARG	A	333	15.752	10.067	0.937	1.00	42.25
AAAAATOM	2455	CB	ARG	A	333	15.212	10.784	-0.306	1.00	43.43
AAAAATOM	2456	CG	ARG	A	333	16.184	11.793	-0.926	1.00	45.99
AAAAATOM	2457	CD	ARG	A	333	15.844	12.060	-2.389	1.00	48.51
AAAAATOM	2458	NE	ARG	A	333	16.415	13.301	-2.913	1.00	50.45
AAAAATOM	2459	CZ	ARG	A	333	17.703	13.631	-2.859	1.00	52.07
AAAAATOM	2460	NH1	ARG	A	333	18.585	12.814	-2.297	1.00	52.45
AAAAATOM	2461	NH2	ARG	A	333	18.112	14.784	-3.377	1.00	51.94
AAAAATOM	2462	C	ARG	A	333	14.594	9.519	1.777	1.00	41.39
AAAAATOM	2463	O	ARG	A	333	14.275	10.060	2.834	1.00	40.21
AAAAATOM	2464	N	ALA	A	334	13.981	8.435	1.308	1.00	40.03
AAAAATOM	2465	CA	ALA	A	334	12.859	7.825	2.014	1.00	39.84
AAAAATOM	2466	CB	ALA	A	334	12.356	6.612	1.241	1.00	38.43
AAAAATOM	2467	C	ALA	A	334	13.239	7.417	3.435	1.00	40.05
AAAAATOM	2468	O	ALA	A	334	12.493	7.665	4.386	1.00	40.41
AAAAATOM	2469	N	ARG	A	335	14.404	6.797	3.577	1.00	39.11
AAAAATOM	2470	CA	ARG	A	335	14.874	6.351	4.881	1.00	40.00
AAAAATOM	2471	CB	ARG	A	335	16.137	5.506	4.719	1.00	39.98
AAAAATOM	2472	CG	ARG	A	335	16.631	4.865	6.000	1.00	40.54
AAAAATOM	2473	CD	ARG	A	335	15.653	3.814	6.501	1.00	42.08
AAAAATOM	2474	NE	ARG	A	335	16.263	2.949	7.507	1.00	42.95
AAAAATOM	2475	CZ	ARG	A	335	16.403	1.634	7.373	1.00	43.43
AAAAATOM	2476	NH1	ARG	A	335	15.972	1.024	6.274	1.00	43.17
AAAAATOM	2477	NH2	ARG	A	335	16.983	0.927	8.335	1.00	43.96
AAAAATOM	2478	C	ARG	A	335	15.167	7.527	5.802	1.00	40.09
AAAAATOM	2479	O	ARG	A	335	14.877	7.479	6.997	1.00	39.35
AAAAATOM	2480	N	ALA	A	336	15.745	8.581	5.237	1.00	40.52
AAAAATOM	2481	CA	ALA	A	336	16.089	9.774	6.001	1.00	41.50
AAAAATOM	2482	CB	ALA	A	336	16.850	10.754	5.116	1.00	41.05
AAAAATOM	2483	C	ALA	A	336	14.847	10.447	6.573	1.00	42.00

AAAAATOM	2484	O	ALA	A	336	14.905	11.087	7.621	1.00 42.49
AAAAATOM	2485	N	ALA	A	337	13.725	10.300	5.879	1.00 42.58
AAAAATOM	2486	CA	ALA	A	337	12.475	10.903	6.320	1.00 42.55
AAAAATOM	2487	CB	ALA	A	337	11.656	11.338	5.111	1.00 42.34
AAAAATOM	2488	C	ALA	A	337	11.670	9.932	7.174	1.00 42.43
AAAAATOM	2489	O	ALA	A	337	10.444	10.000	7.209	1.00 44.01
AAAAATOM	2490	N	SER	A	338	12.360	9.035	7.868	1.00 41.93
AAAAATOM	2491	CA	SER	A	338	11.686	8.053	8.708	1.00 41.12
AAAAATOM	2492	CB	SER	A	338	12.097	6.641	8.293	1.00 40.73
AAAAATOM	2493	OG	SER	A	338	11.504	5.671	9.139	1.00 40.32
AAAAATOM	2494	C	SER	A	338	11.964	8.235	10.198	1.00 40.88
AAAAATOM	2495	O	SER	A	338	13.042	8.674	10.594	1.00 41.46
AAAAATOM	2496	N	ILE	A	339	10.971	7.898	11.013	1.00 40.11
AAAAATOM	2497	CA	ILE	A	339	11.080	7.985	12.461	1.00 39.66
AAAAATOM	2498	CB	ILE	A	339	10.061	8.992	13.038	1.00 39.74
AAAAATOM	2499	CG2	ILE	A	339	10.249	9.118	14.544	1.00 38.88
AAAAATOM	2500	CG1	ILE	A	339	10.249	10.354	12.361	1.00 39.75
AAAAATOM	2501	CD1	ILE	A	339	9.263	11.423	12.804	1.00 40.42
AAAAATOM	2502	C	ILE	A	339	10.788	6.576	12.978	1.00 40.19
AAAAATOM	2503	O	ILE	A	339	9.653	6.102	12.923	1.00 39.97
AAAAATOM	2504	N	PRO	A	340	11.821	5.886	13.484	1.00 40.75
AAAAATOM	2505	CD	PRO	A	340	13.225	6.336	13.448	1.00 40.95
AAAAATOM	2506	CA	PRO	A	340	11.728	4.520	14.012	1.00 40.57
AAAAATOM	2507	CB	PRO	A	340	13.161	4.021	13.877	1.00 41.22
AAAAATOM	2508	CG	PRO	A	340	13.944	5.244	14.222	1.00 41.12
AAAAATOM	2509	C	PRO	A	340	11.180	4.294	15.424	1.00 40.38
AAAAATOM	2510	O	PRO	A	340	10.841	3.163	15.776	1.00 40.48
AAAAATOM	2511	N	ASP	A	341	11.080	5.345	16.232	1.00 39.43
AAAAATOM	2512	CA	ASP	A	341	10.603	5.174	17.603	1.00 38.32
AAAAATOM	2513	CB	ASP	A	341	11.668	5.696	18.578	1.00 38.62
AAAAATOM	2514	CG	ASP	A	341	12.044	7.146	18.317	1.00 39.54
AAAAATOM	2515	OD1	ASP	A	341	11.727	7.658	17.221	1.00 38.30
AAAAATOM	2516	OD2	ASP	A	341	12.668	7.771	19.209	1.00 40.07
AAAAATOM	2517	C	ASP	A	341	9.241	5.789	17.939	1.00 37.27
AAAAATOM	2518	O	ASP	A	341	9.014	6.235	19.066	1.00 35.88
AAAAATOM	2519	N	ALA	A	342	8.329	5.789	16.971	1.00 36.20
AAAAATOM	2520	CA	ALA	A	342	6.996	6.349	17.181	1.00 34.98
AAAAATOM	2521	CB	ALA	A	342	6.150	6.156	15.927	1.00 35.84
AAAAATOM	2522	C	ALA	A	342	6.280	5.744	18.389	1.00 34.17
AAAAATOM	2523	O	ALA	A	342	5.843	6.465	19.289	1.00 33.36
AAAAATOM	2524	N	THR	A	343	6.159	4.421	18.410	1.00 33.49
AAAAATOM	2525	CA	THR	A	343	5.481	3.747	19.512	1.00 33.39
AAAAATOM	2526	CB	THR	A	343	5.567	2.211	19.362	1.00 33.34
AAAAATOM	2527	OG1	THR	A	343	4.951	1.818	18.128	1.00 34.05
AAAAATOM	2528	CG2	THR	A	343	4.851	1.519	20.516	1.00 33.82
AAAAATOM	2529	C	THR	A	343	6.067	4.155	20.865	1.00 33.89
AAAAATOM	2530	O	THR	A	343	5.340	4.591	21.756	1.00 32.15
AAAAATOM	2531	N	GLU	A	344	7.383	4.027	21.007	1.00 34.87
AAAAATOM	2532	CA	GLU	A	344	8.055	4.379	22.257	1.00 35.80
AAAAATOM	2533	CB	GLU	A	344	9.553	4.054	22.177	1.00 37.79
AAAAATOM	2534	CG	GLU	A	344	9.892	2.570	22.029	1.00 41.45
AAAAATOM	2535	CD	GLU	A	344	9.963	2.101	20.581	1.00 44.16
AAAAATOM	2536	OE1	GLU	A	344	10.311	0.917	20.357	1.00 45.57
AAAAATOM	2537	OE2	GLU	A	344	9.676	2.910	19.668	1.00 45.28
AAAAATOM	2538	C	GLU	A	344	7.886	5.856	22.590	1.00 35.95
AAAAATOM	2539	O	GLU	A	344	7.751	6.233	23.754	1.00 35.12
AAAAATOM	2540	N	ARG	A	345	7.896	6.689	21.559	1.00 35.83
AAAAATOM	2541	CA	ARG	A	345	7.759	8.127	21.731	1.00 36.32
AAAAATOM	2542	CB	ARG	A	345	7.999	8.803	20.386	1.00 38.26
AAAAATOM	2543	CG	ARG	A	345	8.268	10.280	20.448	1.00 41.85
AAAAATOM	2544	CD	ARG	A	345	9.006	10.686	19.194	1.00 44.45
AAAAATOM	2545	NE	ARG	A	345	9.194	12.128	19.098	1.00 47.27
AAAAATOM	2546	CZ	ARG	A	345	9.855	12.721	18.111	1.00 47.66
AAAAATOM	2547	NH1	ARG	A	345	10.390	11.988	17.144	1.00 48.37
AAAAATOM	2548	NH2	ARG	A	345	9.974	14.042	18.090	1.00 48.27
AAAAATOM	2549	C	ARG	A	345	6.384	8.510	22.289	1.00 35.99

AAAAATOM	2550	O	ARG	A	345	6.285	9.209	23.302	1.00	35.24
AAAAATOM	2551	N	VAL	A	346	5.324	8.052	21.630	1.00	34.14
AAAAATOM	2552	CA	VAL	A	346	3.975	8.355	22.092	1.00	33.40
AAAAATOM	2553	CB	VAL	A	346	2.909	7.816	21.110	1.00	33.26
AAAAATOM	2554	CG1	VAL	A	346	1.516	7.969	21.709	1.00	33.83
AAAAATOM	2555	CG2	VAL	A	346	3.005	8.565	19.793	1.00	32.47
AAAAATOM	2556	C	VAL	A	346	3.770	7.727	23.466	1.00	33.14
AAAAATOM	2557	O	VAL	A	346	3.172	8.336	24.352	1.00	32.24
AAAAATOM	2558	N	ALA	A	347	4.280	6.510	23.643	1.00	32.01
AAAAATOM	2559	CA	ALA	A	347	4.159	5.813	24.917	1.00	32.80
AAAAATOM	2560	CB	ALA	A	347	4.831	4.447	24.839	1.00	31.97
AAAAATOM	2561	C	ALA	A	347	4.788	6.639	26.031	1.00	33.01
AAAAATOM	2562	O	ALA	A	347	4.214	6.769	27.114	1.00	32.22
AAAAATOM	2563	N	ASN	A	348	5.968	7.193	25.758	1.00	33.65
AAAAATOM	2564	CA	ASN	A	348	6.681	8.009	26.738	1.00	35.77
AAAAATOM	2565	CB	ASN	A	348	8.078	8.382	26.228	1.00	37.45
AAAAATOM	2566	CG	ASN	A	348	8.996	7.183	26.119	1.00	40.90
AAAAATOM	2567	OD1	ASN	A	348	8.998	6.308	26.989	1.00	43.23
AAAAATOM	2568	ND2	ASN	A	348	9.795	7.140	25.057	1.00	42.50
AAAAATOM	2569	C	ASN	A	348	5.912	9.281	27.074	1.00	35.43
AAAAATOM	2570	O	ASN	A	348	5.824	9.662	28.240	1.00	34.83
AAAAATOM	2571	N	GLU	A	349	5.372	9.943	26.051	1.00	35.34
AAAAATOM	2572	CA	GLU	A	349	4.600	11.164	26.264	1.00	34.80
AAAAATOM	2573	CB	GLU	A	349	4.203	11.802	24.932	1.00	36.04
AAAAATOM	2574	CG	GLU	A	349	5.277	12.681	24.323	1.00	38.86
AAAAATOM	2575	CD	GLU	A	349	5.713	13.801	25.257	1.00	40.72
AAAAATOM	2576	OE1	GLU	A	349	4.836	14.458	25.860	1.00	41.85
AAAAATOM	2577	OE2	GLU	A	349	6.933	14.033	25.385	1.00	42.23
AAAAATOM	2578	C	GLU	A	349	3.357	10.863	27.084	1.00	32.75
AAAAATOM	2579	O	GLU	A	349	2.962	11.658	27.932	1.00	32.53
AAAAATOM	2580	N	VAL	A	350	2.737	9.716	26.827	1.00	31.83
AAAAATOM	2581	CA	VAL	A	350	1.556	9.323	27.583	1.00	31.06
AAAAATOM	2582	CB	VAL	A	350	0.952	8.000	27.049	1.00	31.68
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BBBBATOM   2797  CG  HIS B  29       0.177 -34.957 -40.743  1.00 35.61
BBBBATOM   2798  CD2 HIS B  29       0.667 -35.292 -41.960  1.00 36.38
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BBBBATOM	2812	N	MET	B	31	-5.401	-38.168	-41.297	1.00	33.50
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BBBBATOM   2868  N   ARG B  38      -7.629 -46.451 -37.758  1.00 32.20
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BBBBATOM   3006  O   HIS B  54     -10.487 -38.224 -32.620  1.00 34.99
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BBBBATOM   3008  CA  GLY B  55     -12.938 -39.481 -32.447  1.00 35.34
BBBBATOM   3009  C   GLY B  55     -12.427 -40.619 -33.310  1.00 36.18
BBBBATOM   3010  O   GLY B  55     -12.883 -40.799 -34.442  1.00 35.99
BBBBATOM   3011  N   ILE B  56     -11.490 -41.399 -32.776  1.00 35.32
BBBBATOM   3012  CA  ILE B  56     -10.909 -42.517 -33.514  1.00 33.81
BBBBATOM   3013  CB  ILE B  56      -9.374 -42.445 -33.462  1.00 33.36
BBBBATOM   3014  CG2 ILE B  56      -8.761 -43.602 -34.245  1.00 32.87
BBBBATOM   3015  CG1 ILE B  56      -8.916 -41.097 -34.029  1.00 32.05
BBBBATOM   3016  CD1 ILE B  56      -7.461 -40.792 -33.818  1.00 30.35
BBBBATOM   3017  C   ILE B  56     -11.375 -43.859 -32.956  1.00 34.45
BBBBATOM   3018  O   ILE B  56     -11.394 -44.069 -31.738  1.00 34.26
BBBBATOM   3019  N   GLU B  57     -11.764 -44.758 -33.855  1.00 33.40
BBBBATOM   3020  CA  GLU B  57     -12.228 -46.083 -33.467  1.00 34.16
BBBBATOM   3021  CB  GLU B  57     -12.905 -46.769 -34.651  1.00 37.41
BBBBATOM   3022  CG  GLU B  57     -14.064 -45.982 -35.244  1.00 42.10
BBBBATOM   3023  CD  GLU B  57     -14.653 -46.659 -36.465  1.00 45.50
BBBBATOM   3024  OE1 GLU B  57     -13.903 -46.875 -37.448  1.00 46.39
BBBBATOM   3025  OE2 GLU B  57     -15.866 -46.977 -36.441  1.00 48.36
BBBBATOM   3026  C   GLU B  57     -11.044 -46.923 -33.005  1.00 33.01
BBBBATOM   3027  O   GLU B  57      -9.931 -46.769 -33.504  1.00 31.58
BBBBATOM   3028  N   ILE B  58     -11.287 -47.817 -32.056  1.00 31.85
BBBBATOM   3029  CA  ILE B  58     -10.217 -48.658 -31.553  1.00 31.38
BBBBATOM   3030  CB  ILE B  58      -9.651 -48.099 -30.223  1.00 30.95
BBBBATOM   3031  CG2 ILE B  58     -10.769 -47.946 -29.205  1.00 31.48
BBBBATOM   3032  CG1 ILE B  58      -8.553 -49.030 -29.690  1.00 31.13
BBBBATOM   3033  CD1 ILE B  58      -7.736 -48.437 -28.572  1.00 29.87
BBBBATOM   3034  C   ILE B  58     -10.647 -50.102 -31.357  1.00 31.67
BBBBATOM   3035  O   ILE B  58     -11.716 -50.384 -30.801  1.00 30.68
BBBBATOM   3036  N   ASP B  59      -9.807 -51.011 -31.844  1.00 30.76
BBBBATOM   3037  CA  ASP B  59     -10.039 -52.442 -31.720  1.00 31.09
BBBBATOM   3038  CB  ASP B  59      -9.732 -53.153 -33.037  1.00 31.37
BBBBATOM   3039  CG  ASP B  59     -10.766 -52.863 -34.104  1.00 32.68
BBBBATOM   3040  OD1 ASP B  59     -11.969 -53.037 -33.812  1.00 32.40
BBBBATOM   3041  OD2 ASP B  59     -10.378 -52.468 -35.224  1.00 33.40
BBBBATOM   3042  C   ASP B  59      -9.119 -52.950 -30.618  1.00 30.50
BBBBATOM   3043  O   ASP B  59      -7.987 -52.491 -30.492  1.00 30.24
BBBBATOM   3044  N   PHE B  60      -9.608 -53.888 -29.815  1.00 30.65
BBBBATOM   3045  CA  PHE B  60      -8.809 -54.410 -28.713  1.00 30.32
BBBBATOM   3046  CB  PHE B  60      -9.560 -54.239 -27.385  1.00 30.74
BBBBATOM   3047  CG  PHE B  60      -9.925 -52.815 -27.058  1.00 32.14
BBBBATOM   3048  CD1 PHE B  60     -11.250 -52.392 -27.129  1.00 33.15
BBBBATOM   3049  CD2 PHE B  60      -8.955 -51.908 -26.649  1.00 31.57
BBBBATOM   3050  CE1 PHE B  60     -11.605 -51.083 -26.791  1.00 34.05
BBBBATOM   3051  CE2 PHE B  60      -9.294 -50.598 -26.310  1.00 33.00
BBBBATOM   3052  CZ  PHE B  60     -10.626 -50.185 -26.380  1.00 33.82
BBBBATOM   3053  C   PHE B  60      -8.430 -55.878 -28.846  1.00 29.86
BBBBATOM   3054  O   PHE B  60      -9.154 -56.668 -29.445  1.00 29.93
BBBBATOM   3055  N   ILE B  61      -7.271 -56.229 -28.295  1.00 29.38
BBBBATOM   3056  CA  ILE B  61      -6.832 -57.616 -28.269  1.00 28.55
BBBBATOM   3057  CB  ILE B  61      -5.674 -57.923 -29.258  1.00 28.48
BBBBATOM   3058  CG2 ILE B  61      -6.123 -57.650 -30.694  1.00 27.65
BBBBATOM   3059  CG1 ILE B  61      -4.422 -57.126 -28.892  1.00 26.70
BBBBATOM   3060  CD1 ILE B  61      -3.177 -57.615 -29.638  1.00 27.03
BBBBATOM   3061  C   ILE B  61      -6.344 -57.855 -26.848  1.00 29.13
BBBBATOM   3062  O   ILE B  61      -6.124 -56.906 -26.091  1.00 28.80
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BBBBATOM	3063	N	ARG	B	62	-6.186	-59.116	-26.473	1.00 29.38
BBBBATOM	3064	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00 30.76
BBBBATOM	3065	CB	ARG	B	62	-6.630	-60.447	-24.461	1.00 32.36
BBBBATOM	3066	CG	ARG	B	62	-6.130	-60.955	-23.114	1.00 35.99
BBBBATOM	3067	CD	ARG	B	62	-5.438	-59.859	-22.311	1.00 37.86
BBBBATOM	3068	NE	ARG	B	62	-6.297	-58.718	-22.004	1.00 40.01
BBBBATOM	3069	CZ	ARG	B	62	-5.840	-57.504	-21.711	1.00 39.09
BBBBATOM	3070	NH1	ARG	B	62	-4.536	-57.275	-21.690	1.00 39.24
BBBBATOM	3071	NH2	ARG	B	62	-6.686	-56.518	-21.439	1.00 40.03
BBBBATOM	3072	C	ARG	B	62	-4.274	-59.923	-25.156	1.00 29.32
BBBBATOM	3073	O	ARG	B	62	-3.933	-60.809	-25.934	1.00 28.65
BBBBATOM	3074	N	ILE	B	63	-3.428	-59.342	-24.313	1.00 30.07
BBBBATOM	3075	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00 31.38
BBBBATOM	3076	CB	ILE	B	63	-1.081	-58.745	-24.883	1.00 30.06
BBBBATOM	3077	CG2	ILE	B	63	-1.442	-58.567	-26.353	1.00 30.41
BBBBATOM	3078	CG1	ILE	B	63	-1.143	-57.411	-24.137	1.00 29.94
BBBBATOM	3079	CD1	ILE	B	63	-0.128	-56.384	-24.632	1.00 29.62
BBBBATOM	3080	C	ILE	B	63	-1.623	-59.981	-22.775	1.00 33.08
BBBBATOM	3081	O	ILE	B	63	-0.444	-59.872	-22.430	1.00 33.21
BBBBATOM	3082	N	SER	B	64	-2.603	-60.284	-21.927	1.00 35.38
BBBBATOM	3083	CA	SER	B	64	-2.356	-60.520	-20.505	1.00 37.51
BBBBATOM	3084	CB	SER	B	64	-3.652	-60.912	-19.792	1.00 38.82
BBBBATOM	3085	OG	SER	B	64	-4.558	-59.823	-19.750	1.00 42.88
BBBBATOM	3086	C	SER	B	64	-1.326	-61.622	-20.311	1.00 37.32
BBBBATOM	3087	O	SER	B	64	-1.411	-62.682	-20.933	1.00 37.86
BBBBATOM	3088	N	GLY	B	65	-0.356	-61.370	-19.441	1.00 37.81
BBBBATOM	3089	CA	GLY	B	65	0.679	-62.355	-19.199	1.00 37.13
BBBBATOM	3090	C	GLY	B	65	1.798	-62.283	-20.226	1.00 36.76
BBBBATOM	3091	O	GLY	B	65	2.858	-62.889	-20.038	1.00 37.57
BBBBATOM	3092	N	LEU	B	66	1.577	-61.539	-21.307	1.00 34.63
BBBBATOM	3093	CA	LEU	B	66	2.591	-61.413	-22.355	1.00 33.17
BBBBATOM	3094	CB	LEU	B	66	1.936	-61.470	-23.735	1.00 32.08
BBBBATOM	3095	CG	LEU	B	66	1.162	-62.747	-24.061	1.00 32.52
BBBBATOM	3096	CD1	LEU	B	66	0.563	-62.626	-25.445	1.00 31.38
BBBBATOM	3097	CD2	LEU	B	66	2.093	-63.957	-23.984	1.00 31.67
BBBBATOM	3098	C	LEU	B	66	3.414	-60.133	-22.246	1.00 32.72
BBBBATOM	3099	O	LEU	B	66	4.451	-60.002	-22.893	1.00 33.13
BBBBATOM	3100	N	ARG	B	67	2.953	-59.185	-21.440	1.00 31.54
BBBBATOM	3101	CA	ARG	B	67	3.671	-57.928	-21.277	1.00 30.90
BBBBATOM	3102	CB	ARG	B	67	2.888	-56.984	-20.363	1.00 32.28
BBBBATOM	3103	CG	ARG	B	67	1.540	-56.576	-20.913	1.00 34.65
BBBBATOM	3104	CD	ARG	B	67	0.926	-55.440	-20.097	1.00 36.69
BBBBATOM	3105	NE	ARG	B	67	-0.259	-54.889	-20.748	1.00 38.28
BBBBATOM	3106	CZ	ARG	B	67	-1.425	-55.519	-20.853	1.00 39.05
BBBBATOM	3107	NH1	ARG	B	67	-1.583	-56.734	-20.341	1.00 39.61
BBBBATOM	3108	NH2	ARG	B	67	-2.434	-54.935	-21.487	1.00 39.52
BBBBATOM	3109	C	ARG	B	67	5.071	-58.142	-20.713	1.00 29.99
BBBBATOM	3110	O	ARG	B	67	5.294	-59.034	-19.889	1.00 28.67
BBBBATOM	3111	N	GLY	B	68	6.014	-57.321	-21.165	1.00 27.75
BBBBATOM	3112	CA	GLY	B	68	7.380	-57.427	-20.685	1.00 26.79
BBBBATOM	3113	C	GLY	B	68	8.166	-58.579	-21.280	1.00 25.41
BBBBATOM	3114	O	GLY	B	68	9.326	-58.779	-20.943	1.00 26.04
BBBBATOM	3115	N	LYS	B	69	7.546	-59.342	-22.170	1.00 24.55
BBBBATOM	3116	CA	LYS	B	69	8.238	-60.463	-22.796	1.00 23.93
BBBBATOM	3117	CB	LYS	B	69	7.284	-61.641	-23.033	1.00 24.12
BBBBATOM	3118	CG	LYS	B	69	6.757	-62.360	-21.794	1.00 25.08
BBBBATOM	3119	CD	LYS	B	69	5.887	-63.553	-22.224	1.00 25.44
BBBBATOM	3120	CE	LYS	B	69	5.357	-64.358	-21.035	1.00 28.31
BBBBATOM	3121	NZ	LYS	B	69	6.468	-64.877	-20.175	1.00 29.71
BBBBATOM	3122	C	LYS	B	69	8.825	-60.062	-24.142	1.00 23.32
BBBBATOM	3123	O	LYS	B	69	8.151	-59.404	-24.944	1.00 21.96
BBBBATOM	3124	N	GLY	B	70	10.075	-60.470	-24.374	1.00 22.48
BBBBATOM	3125	CA	GLY	B	70	10.755	-60.229	-25.636	1.00 22.26
BBBBATOM	3126	C	GLY	B	70	10.308	-61.337	-26.588	1.00 22.17
BBBBATOM	3127	O	GLY	B	70	9.512	-62.183	-26.195	1.00 21.62
BBBBATOM	3128	N	ILE	B	71	10.819	-61.373	-27.814	1.00 21.85

BBBBATOM	3129	CA	ILE	B	71	10.357	-62.386	-28.762	1.00	23.55
BBBBATOM	3130	CB	ILE	B	71	10.926	-62.142	-30.181	1.00	23.52
BBBBATOM	3131	CG2	ILE	B	71	12.435	-62.375	-30.192	1.00	25.96
BBBBATOM	3132	CG1	ILE	B	71	10.264	-63.096	-31.182	1.00	24.18
BBBBATOM	3133	CD1	ILE	B	71	8.745	-62.981	-31.263	1.00	25.73
BBBBATOM	3134	C	ILE	B	71	10.616	-63.840	-28.359	1.00	23.88
BBBBATOM	3135	O	ILE	B	71	9.775	-64.707	-28.592	1.00	21.66
BBBBATOM	3136	N	LYS	B	72	11.764	-64.119	-27.751	1.00	23.82
BBBBATOM	3137	CA	LYS	B	72	12.038	-65.491	-27.343	1.00	24.92
BBBBATOM	3138	CB	LYS	B	72	13.491	-65.634	-26.875	1.00	26.86
BBBBATOM	3139	CG	LYS	B	72	14.496	-65.590	-28.019	1.00	31.29
BBBBATOM	3140	CD	LYS	B	72	15.925	-65.791	-27.518	1.00	36.00
BBBBATOM	3141	CE	LYS	B	72	16.926	-65.816	-28.671	1.00	38.82
BBBBATOM	3142	NZ	LYS	B	72	18.342	-65.957	-28.192	1.00	41.21
BBBBATOM	3143	C	LYS	B	72	11.068	-65.925	-26.245	1.00	23.73
BBBBATOM	3144	O	LYS	B	72	10.592	-67.062	-26.245	1.00	24.08
BBBBATOM	3145	N	ALA	B	73	10.765	-65.016	-25.322	1.00	21.62
BBBBATOM	3146	CA	ALA	B	73	9.839	-65.306	-24.233	1.00	21.18
BBBBATOM	3147	CB	ALA	B	73	9.895	-64.196	-23.187	1.00	22.25
BBBBATOM	3148	C	ALA	B	73	8.412	-65.454	-24.771	1.00	20.36
BBBBATOM	3149	O	ALA	B	73	7.619	-66.250	-24.267	1.00	18.97
BBBBATOM	3150	N	LEU	B	74	8.076	-64.673	-25.791	1.00	20.23
BBBBATOM	3151	CA	LEU	B	74	6.745	-64.762	-26.387	1.00	19.36
BBBBATOM	3152	CB	LEU	B	74	6.540	-63.643	-27.417	1.00	18.42
BBBBATOM	3153	CG	LEU	B	74	6.422	-62.208	-26.884	1.00	18.80
BBBBATOM	3154	CD1	LEU	B	74	6.473	-61.197	-28.039	1.00	19.86
BBBBATOM	3155	CD2	LEU	B	74	5.109	-62.071	-26.104	1.00	19.45
BBBBATOM	3156	C	LEU	B	74	6.549	-66.110	-27.069	1.00	19.37
BBBBATOM	3157	O	LEU	B	74	5.539	-66.779	-26.863	1.00	20.01
BBBBATOM	3158	N	ILE	B	75	7.520	-66.507	-27.883	1.00	20.59
BBBBATOM	3159	CA	ILE	B	75	7.434	-67.768	-28.601	1.00	21.18
BBBBATOM	3160	CB	ILE	B	75	8.571	-67.896	-29.641	1.00	22.95
BBBBATOM	3161	CG2	ILE	B	75	8.334	-69.108	-30.527	1.00	25.38
BBBBATOM	3162	CG1	ILE	B	75	8.598	-66.657	-30.540	1.00	26.82
BBBBATOM	3163	CD1	ILE	B	75	7.304	-66.442	-31.327	1.00	28.48
BBBBATOM	3164	C	ILE	B	75	7.488	-68.942	-27.624	1.00	21.20
BBBBATOM	3165	O	ILE	B	75	7.125	-70.063	-27.979	1.00	21.59
BBBBATOM	3166	N	ALA	B	76	7.940	-68.680	-26.399	1.00	20.49
BBBBATOM	3167	CA	ALA	B	76	7.996	-69.726	-25.374	1.00	21.72
BBBBATOM	3168	CB	ALA	B	76	9.026	-69.372	-24.305	1.00	21.92
BBBBATOM	3169	C	ALA	B	76	6.624	-69.904	-24.732	1.00	21.54
BBBBATOM	3170	O	ALA	B	76	6.441	-70.778	-23.875	1.00	20.75
BBBBATOM	3171	N	ALA	B	77	5.668	-69.066	-25.145	1.00	20.61
BBBBATOM	3172	CA	ALA	B	77	4.289	-69.121	-24.655	1.00	21.07
BBBBATOM	3173	CB	ALA	B	77	3.937	-67.830	-23.924	1.00	20.10
BBBBATOM	3174	C	ALA	B	77	3.383	-69.298	-25.881	1.00	21.69
BBBBATOM	3175	O	ALA	B	77	2.567	-68.430	-26.199	1.00	21.93
BBBBATOM	3176	N	PRO	B	78	3.507	-70.446	-26.564	1.00	22.38
BBBBATOM	3177	CD	PRO	B	78	4.211	-71.603	-25.976	1.00	21.89
BBBBATOM	3178	CA	PRO	B	78	2.772	-70.846	-27.771	1.00	20.95
BBBBATOM	3179	CB	PRO	B	78	3.027	-72.350	-27.861	1.00	22.21
BBBBATOM	3180	CG	PRO	B	78	4.288	-72.547	-27.117	1.00	24.07
BBBBATOM	3181	C	PRO	B	78	1.278	-70.535	-27.813	1.00	21.19
BBBBATOM	3182	O	PRO	B	78	0.789	-69.939	-28.776	1.00	19.68
BBBBATOM	3183	N	LEU	B	79	0.544	-70.961	-26.790	1.00	21.21
BBBBATOM	3184	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00	21.32
BBBBATOM	3185	CB	LEU	B	79	-1.569	-71.476	-25.630	1.00	20.99
BBBBATOM	3186	CG	LEU	B	79	-1.397	-72.988	-25.617	1.00	22.40
BBBBATOM	3187	CD1	LEU	B	79	-2.504	-73.619	-24.772	1.00	22.01
BBBBATOM	3188	CD2	LEU	B	79	-1.438	-73.521	-27.021	1.00	23.82
BBBBATOM	3189	C	LEU	B	79	-1.275	-69.263	-26.707	1.00	21.17
BBBBATOM	3190	O	LEU	B	79	-2.125	-68.800	-27.481	1.00	20.44
BBBBATOM	3191	N	ARG	B	80	-0.656	-68.529	-25.788	1.00	20.91
BBBBATOM	3192	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00	21.30
BBBBATOM	3193	CB	ARG	B	80	-0.444	-66.583	-24.312	1.00	22.12
BBBBATOM	3194	CG	ARG	B	80	-1.286	-67.051	-23.118	1.00	24.03

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BBBBATOM   3195  CD  ARG B  80      -0.610 -66.738 -21.807  1.00 23.42
BBBBATOM   3196  NE  ARG B  80       0.581 -67.556 -21.610  1.00 24.59
BBBBATOM   3197  CZ  ARG B  80       1.466 -67.351 -20.642  1.00 26.08
BBBBATOM   3198  NH1 ARG B  80       1.290 -66.349 -19.787  1.00 26.92
BBBBATOM   3199  NH2 ARG B  80       2.514 -68.152 -20.519  1.00 27.22
BBBBATOM   3200  C   ARG B  80      -0.526 -66.233 -26.790  1.00 21.29
BBBBATOM   3201  O   ARG B  80      -1.278 -65.355 -27.223  1.00 21.47
BBBBATOM   3202  N   ILE B  81       0.683 -66.448 -27.303  1.00 19.29
BBBBATOM   3203  CA  ILE B  81       1.113 -65.621 -28.421  1.00 19.47
BBBBATOM   3204  CB  ILE B  81       2.639 -65.793 -28.730  1.00 17.92
BBBBATOM   3205  CG2 ILE B  81       2.949 -67.200 -29.206  1.00 17.33
BBBBATOM   3206  CG1 ILE B  81       3.067 -64.753 -29.769  1.00 18.63
BBBBATOM   3207  CD1 ILE B  81       2.746 -63.318 -29.346  1.00 17.46
BBBBATOM   3208  C   ILE B  81       0.256 -65.937 -29.654  1.00 18.99
BBBBATOM   3209  O   ILE B  81      -0.149 -65.028 -30.378  1.00 19.38
BBBBATOM   3210  N   PHE B  82      -0.056 -67.211 -29.880  1.00 19.39
BBBBATOM   3211  CA  PHE B  82      -0.875 -67.582 -31.038  1.00 19.15
BBBBATOM   3212  CB  PHE B  82      -1.057 -69.103 -31.136  1.00 19.27
BBBBATOM   3213  CG  PHE B  82      -1.811 -69.548 -32.368  1.00 19.87
BBBBATOM   3214  CD1 PHE B  82      -1.180 -69.602 -33.603  1.00 20.87
BBBBATOM   3215  CD2 PHE B  82      -3.154 -69.898 -32.289  1.00 21.11
BBBBATOM   3216  CE1 PHE B  82      -1.872 -70.002 -34.753  1.00 21.20
BBBBATOM   3217  CE2 PHE B  82      -3.857 -70.297 -33.429  1.00 22.26
BBBBATOM   3218  CZ  PHE B  82      -3.212 -70.349 -34.663  1.00 22.14
BBBBATOM   3219  C   PHE B  82      -2.250 -66.931 -30.959  1.00 19.94
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BBBBATOM   3221  N   ASN B  83      -2.832 -66.923 -29.764  1.00 19.29
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BBBBATOM   3223  CB  ASN B  83      -4.693 -66.641 -28.178  1.00 20.55
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BBBBATOM   3249  CA  ARG B  86      -5.140 -64.660 -34.166  1.00 23.28
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BBBBATOM	3449	N	ALA	B	114	0.875	-60.010	-36.892	1.00 18.96
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BBBBATOM   3481  CB  LEU B 118      -2.195 -60.155 -43.227  1.00 25.80
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BBBBATOM   3491  N   ILE B 120       0.786 -57.173 -44.940  1.00 25.88
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BBBBATOM   3508  CB  VAL B 122       5.184 -53.694 -40.095  1.00 21.80
BBBBATOM   3509  CG1 VAL B 122       5.426 -53.085 -38.724  1.00 21.97
BBBBATOM   3510  CG2 VAL B 122       4.133 -54.789 -40.035  1.00 22.19
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BBBBATOM   3516  CG1 VAL B 123       6.516 -46.722 -40.709  1.00 20.83
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BBBBATOM   3650  NZ   LYS B 140      17.692 -59.713 -34.320  1.00 36.17
BBBBATOM   3651  C    LYS B 140      12.254 -57.833 -39.212  1.00 27.83
BBBBATOM   3652  O    LYS B 140      12.602 -58.562 -40.142  1.00 27.80
BBBBATOM   3653  N    ILE B 141      10.992 -57.445 -39.052  1.00 26.40
BBBBATOM   3654  CA   ILE B 141       9.963 -57.818 -40.016  1.00 26.09
BBBBATOM   3655  CB   ILE B 141       8.854 -58.721 -39.405  1.00 26.39
BBBBATOM   3656  CG2  ILE B 141       9.401 -60.118 -39.145  1.00 28.33
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BBBBATOM	3657	CG1	ILE	B	141	8.298	-58.092	-38.127	1.00	26.45
BBBBATOM	3658	CD1	ILE	B	141	7.136	-58.845	-37.549	1.00	26.95
BBBBATOM	3659	C	ILE	B	141	9.316	-56.542	-40.530	1.00	25.81
BBBBATOM	3660	O	ILE	B	141	8.353	-56.586	-41.305	1.00	26.10
BBBBATOM	3661	N	ALA	B	142	9.856	-55.405	-40.097	1.00	23.78
BBBBATOM	3662	CA	ALA	B	142	9.331	-54.107	-40.498	1.00	25.03
BBBBATOM	3663	CB	ALA	B	142	9.717	-53.046	-39.466	1.00	24.89
BBBBATOM	3664	C	ALA	B	142	9.816	-53.680	-41.880	1.00	25.08
BBBBATOM	3665	O	ALA	B	142	10.973	-53.894	-42.237	1.00	24.93
BBBBATOM	3666	N	THR	B	143	8.920	-53.075	-42.651	1.00	25.03
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BBBBATOM	3668	CB	THR	B	143	7.987	-52.318	-44.816	1.00	25.75
BBBBATOM	3669	OG1	THR	B	143	7.249	-53.534	-44.970	1.00	25.54
BBBBATOM	3670	CG2	THR	B	143	8.345	-51.782	-46.207	1.00	26.92
BBBBATOM	3671	C	THR	B	143	10.079	-51.310	-43.863	1.00	26.63
BBBBATOM	3672	O	THR	B	143	10.996	-51.061	-44.656	1.00	27.13
BBBBATOM	3673	N	LYS	B	144	9.753	-50.506	-42.853	1.00	24.95
BBBBATOM	3674	CA	LYS	B	144	10.436	-49.238	-42.618	1.00	24.73
BBBBATOM	3675	CB	LYS	B	144	9.688	-48.103	-43.329	1.00	26.20
BBBBATOM	3676	CG	LYS	B	144	10.202	-46.710	-43.013	1.00	27.44
BBBBATOM	3677	CD	LYS	B	144	11.602	-46.480	-43.558	1.00	29.01
BBBBATOM	3678	CE	LYS	B	144	12.055	-45.051	-43.293	1.00	29.74
BBBBATOM	3679	NZ	LYS	B	144	13.406	-44.774	-43.854	1.00	31.29
BBBBATOM	3680	C	LYS	B	144	10.506	-48.943	-41.125	1.00	24.61
BBBBATOM	3681	O	LYS	B	144	9.493	-49.008	-40.423	1.00	23.36
BBBBATOM	3682	N	VAL	B	145	11.707	-48.623	-40.656	1.00	23.68
BBBBATOM	3683	CA	VAL	B	145	11.947	-48.311	-39.252	1.00	23.62
BBBBATOM	3684	CB	VAL	B	145	12.981	-49.279	-38.617	1.00	23.66
BBBBATOM	3685	CG1	VAL	B	145	13.083	-49.014	-37.114	1.00	24.44
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BBBBATOM	3687	C	VAL	B	145	12.510	-46.900	-39.125	1.00	24.09
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BBBBATOM	3689	N	MET	B	146	11.902	-46.103	-38.251	1.00	23.84
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BBBBATOM	3691	CB	MET	B	146	11.274	-43.729	-38.448	1.00	24.72
BBBBATOM	3692	CG	MET	B	146	11.130	-43.577	-39.970	1.00	21.76
BBBBATOM	3693	SD	MET	B	146	9.649	-42.636	-40.468	1.00	25.05
BBBBATOM	3694	CE	MET	B	146	8.376	-43.846	-40.325	1.00	21.96
BBBBATOM	3695	C	MET	B	146	12.567	-44.593	-36.488	1.00	24.69
BBBBATOM	3696	O	MET	B	146	11.963	-45.311	-35.689	1.00	22.43
BBBBATOM	3697	N	GLN	B	147	13.456	-43.678	-36.112	1.00	23.37
BBBBATOM	3698	CA	GLN	B	147	13.762	-43.418	-34.712	1.00	25.05
BBBBATOM	3699	CB	GLN	B	147	15.067	-44.114	-34.301	1.00	24.99
BBBBATOM	3700	CG	GLN	B	147	16.259	-43.750	-35.169	1.00	26.10
BBBBATOM	3701	CD	GLN	B	147	17.527	-44.508	-34.803	1.00	26.65
BBBBATOM	3702	OE1	GLN	B	147	18.425	-44.671	-35.637	1.00	28.62
BBBBATOM	3703	NE2	GLN	B	147	17.615	-44.966	-33.558	1.00	26.05
BBBBATOM	3704	C	GLN	B	147	13.880	-41.911	-34.515	1.00	26.28
BBBBATOM	3705	O	GLN	B	147	14.292	-41.177	-35.430	1.00	25.02
BBBBATOM	3706	N	ALA	B	148	13.518	-41.452	-33.323	1.00	26.58
BBBBATOM	3707	CA	ALA	B	148	13.559	-40.032	-33.009	1.00	26.88
BBBBATOM	3708	CB	ALA	B	148	12.853	-39.776	-31.685	1.00	26.71
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BBBBATOM	3710	O	ALA	B	148	15.293	-38.463	-33.545	1.00	27.38
BBBBATOM	3711	N	PHE	B	149	15.847	-40.219	-32.242	1.00	27.92
BBBBATOM	3712	CA	PHE	B	149	17.239	-39.820	-32.098	1.00	29.39
BBBBATOM	3713	CB	PHE	B	149	17.596	-39.631	-30.617	1.00	28.95
BBBBATOM	3714	CG	PHE	B	149	16.549	-38.910	-29.821	1.00	28.91
BBBBATOM	3715	CD1	PHE	B	149	15.745	-39.603	-28.929	1.00	27.96
BBBBATOM	3716	CD2	PHE	B	149	16.372	-37.537	-29.957	1.00	29.03
BBBBATOM	3717	CE1	PHE	B	149	14.779	-38.945	-28.178	1.00	28.64
BBBBATOM	3718	CE2	PHE	B	149	15.406	-36.866	-29.211	1.00	30.10
BBBBATOM	3719	CZ	PHE	B	149	14.608	-37.575	-28.317	1.00	29.02
BBBBATOM	3720	C	PHE	B	149	18.153	-40.893	-32.673	1.00	30.03
BBBBATOM	3721	O	PHE	B	149	17.750	-42.036	-32.849	1.00	30.05
BBBBATOM	3722	N	PRO	B	150	19.401	-40.530	-32.991	1.00	31.73

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BBBBATOM   3724  CA  PRO B 150      20.310 -41.541 -33.535  1.00 31.87
BBBBATOM   3725  CB  PRO B 150      21.418 -40.698 -34.154  1.00 33.07
BBBBATOM   3726  CG  PRO B 150      21.480 -39.517 -33.238  1.00 33.70
BBBBATOM   3727  C   PRO B 150      20.809 -42.411 -32.376  1.00 31.93
BBBBATOM   3728  O   PRO B 150      20.873 -41.945 -31.239  1.00 31.39
BBBBATOM   3729  N   GLY B 151      21.130 -43.671 -32.651  1.00 31.67
BBBBATOM   3730  CA  GLY B 151      21.629 -44.537 -31.595  1.00 32.62
BBBBATOM   3731  C   GLY B 151      20.717 -45.655 -31.112  1.00 32.88
BBBBATOM   3732  O   GLY B 151      21.206 -46.690 -30.657  1.00 32.98
BBBBATOM   3733  N   ALA B 152      19.403 -45.458 -31.196  1.00 32.24
BBBBATOM   3734  CA  ALA B 152      18.447 -46.476 -30.753  1.00 32.71
BBBBATOM   3735  CB  ALA B 152      17.020 -45.924 -30.817  1.00 31.78
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BBBBATOM   3738  N   PHE B 153      18.732 -47.462 -32.941  1.00 33.66
BBBBATOM   3739  CA  PHE B 153      18.925 -48.506 -33.937  1.00 34.83
BBBBATOM   3740  CB  PHE B 153      17.734 -48.611 -34.893  1.00 33.64
BBBBATOM   3741  CG  PHE B 153      16.518 -49.244 -34.289  1.00 32.97
BBBBATOM   3742  CD1 PHE B 153      15.468 -48.461 -33.823  1.00 31.93
BBBBATOM   3743  CD2 PHE B 153      16.421 -50.628 -34.184  1.00 32.46
BBBBATOM   3744  CE1 PHE B 153      14.339 -49.049 -33.265  1.00 32.18
BBBBATOM   3745  CE2 PHE B 153      15.294 -51.224 -33.626  1.00 31.75
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BBBBATOM   3749  N   PRO B 154      20.944 -49.040 -35.220  1.00 38.15
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BBBBATOM   3755  O   PRO B 154      22.697 -46.958 -37.496  1.00 39.89
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BBBBATOM   3760  OD1 ASN B 155      23.401 -47.861 -40.922  1.00 46.41
BBBBATOM   3761  ND2 ASN B 155      23.019 -49.978 -40.259  1.00 45.20
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BBBBATOM   3764  N   ALA B 156      18.507 -46.956 -38.638  1.00 38.93
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BBBBATOM   3785  N   VAL B 159      14.186 -39.241 -37.544  1.00 28.57
BBBBATOM   3786  CA  VAL B 159      13.155 -38.265 -37.889  1.00 28.10
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BBBBATOM	3789	CG2	VAL	B	159	11.336	-39.962	-37.548	1.00	27.61
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BBBBATOM	3824	CZ	ARG	B	164	2.307	-26.919	-25.144	1.00	45.79
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BBBBATOM	3826	NH2	ARG	B	164	1.769	-25.705	-25.123	1.00	47.50
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BBBBATOM   3862  C   ALA B 169      7.472 -20.427 -33.078  1.00 32.03
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BBBBATOM   3875  CB  PRO B 171     11.665 -16.054 -32.033  1.00 29.54
BBBBATOM   3876  CG  PRO B 171     10.261 -15.810 -31.605  1.00 30.96
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BBBBATOM   3878  O   PRO B 171     12.999 -18.933 -31.363  1.00 30.16
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BBBBATOM   3880  CA  LEU B 172     15.157 -18.780 -33.062  1.00 28.33
BBBBATOM   3881  CB  LEU B 172     16.106 -18.557 -34.247  1.00 29.88
BBBBATOM   3882  CG  LEU B 172     15.800 -19.149 -35.628  1.00 32.18
BBBBATOM   3883  CD1 LEU B 172     15.593 -20.656 -35.510  1.00 32.75
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BBBBATOM   3885  C   LEU B 172     15.805 -18.206 -31.805  1.00 26.61
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BBBBATOM   3887  N   PRO B 173     16.735 -18.959 -31.190  1.00 25.73
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BBBBATOM   3899  OE1 GLN B 174     20.634 -11.732 -32.491  1.00 26.98
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BBBBATOM   3912  N   ARG B 176     15.288 -14.578 -29.818  1.00 28.19
BBBBATOM   3913  CA  ARG B 176     14.611 -14.635 -28.525  1.00 29.01
BBBBATOM   3914  CB  ARG B 176     14.183 -16.088 -28.260  1.00 32.12
BBBBATOM   3915  CG  ARG B 176     13.783 -16.410 -26.825  1.00 34.95
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BBBBATOM   3918  CZ  ARG B 176     14.458 -19.480 -27.231  1.00 40.44
BBBBATOM   3919  NH1 ARG B 176     15.121 -19.233 -26.107  1.00 41.22
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BBBBATOM   4002  C   LEU B 187      12.450 -24.146 -15.085  1.00 16.85
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BBBBATOM   4004  N   VAL B 188      11.788 -24.426 -13.964  1.00 18.20
BBBBATOM   4005  CA  VAL B 188      11.774 -25.775 -13.381  1.00 18.41
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BBBBATOM   4009  C   VAL B 188      10.434 -26.440 -13.739  1.00 19.88
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BBBBATOM   4026  N   SER B 192       2.587 -32.673 -14.779  1.00 34.23
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BBBBATOM   4050  N   ARG B 196       9.195 -34.592  -7.426  1.00 32.81
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BBBBATOM	4056	CZ	ARG	B	196	8.661	-37.955	-8.997	1.00	42.91
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BBBBATOM	4078	CA	ASN	B	199	10.497	-29.447	-5.563	1.00	27.07
BBBBATOM	4079	CB	ASN	B	199	9.123	-30.035	-5.238	1.00	26.63
BBBBATOM	4080	CG	ASN	B	199	8.212	-30.050	-6.434	1.00	27.62
BBBBATOM	4081	OD1	ASN	B	199	8.519	-29.434	-7.460	1.00	26.33
BBBBATOM	4082	ND2	ASN	B	199	7.080	-30.749	-6.320	1.00	24.20
BBBBATOM	4083	C	ASN	B	199	11.308	-29.319	-4.282	1.00	27.65
BBBBATOM	4084	O	ASN	B	199	11.207	-28.321	-3.581	1.00	28.19
BBBBATOM	4085	N	GLN	B	200	12.124	-30.328	-3.994	1.00	28.38
BBBBATOM	4086	CA	GLN	B	200	12.955	-30.326	-2.794	1.00	30.10
BBBBATOM	4087	CB	GLN	B	200	13.158	-31.764	-2.301	1.00	31.91
BBBBATOM	4088	CG	GLN	B	200	11.883	-32.453	-1.827	1.00	35.02
BBBBATOM	4089	CD	GLN	B	200	12.056	-33.956	-1.632	1.00	37.49
BBBBATOM	4090	OE1	GLN	B	200	11.204	-34.619	-1.032	1.00	38.76
BBBBATOM	4091	NE2	GLN	B	200	13.155	-34.502	-2.151	1.00	37.28
BBBBATOM	4092	C	GLN	B	200	14.319	-29.675	-3.011	1.00	30.18
BBBBATOM	4093	O	GLN	B	200	14.834	-28.975	-2.135	1.00	31.13
BBBBATOM	4094	N	THR	B	201	14.897	-29.884	-4.187	1.00	28.94
BBBBATOM	4095	CA	THR	B	201	16.215	-29.345	-4.474	1.00	27.34
BBBBATOM	4096	CB	THR	B	201	16.915	-30.181	-5.567	1.00	28.81
BBBBATOM	4097	OG1	THR	B	201	16.988	-31.553	-5.149	1.00	28.92
BBBBATOM	4098	CG2	THR	B	201	18.331	-29.654	-5.817	1.00	28.29
BBBBATOM	4099	C	THR	B	201	16.313	-27.871	-4.869	1.00	25.78
BBBBATOM	4100	O	THR	B	201	17.137	-27.138	-4.331	1.00	24.91
BBBBATOM	4101	N	MET	B	202	15.479	-27.430	-5.800	1.00	24.08
BBBBATOM	4102	CA	MET	B	202	15.567	-26.048	-6.268	1.00	23.68
BBBBATOM	4103	CB	MET	B	202	14.558	-25.827	-7.397	1.00	22.29
BBBBATOM	4104	CG	MET	B	202	14.856	-26.685	-8.633	1.00	22.80
BBBBATOM	4105	SD	MET	B	202	16.590	-26.614	-9.190	1.00	25.93
BBBBATOM	4106	CE	MET	B	202	16.814	-24.877	-9.345	1.00	22.63
BBBBATOM	4107	C	MET	B	202	15.489	-24.926	-5.229	1.00	23.47
BBBBATOM	4108	O	MET	B	202	16.189	-23.929	-5.354	1.00	24.40
BBBBATOM	4109	N	PRO	B	203	14.636	-25.059	-4.192	1.00	24.12
BBBBATOM	4110	CD	PRO	B	203	13.518	-25.991	-3.970	1.00	22.27
BBBBATOM	4111	CA	PRO	B	203	14.608	-23.963	-3.220	1.00	23.84
BBBBATOM	4112	CB	PRO	B	203	13.553	-24.424	-2.217	1.00	24.46
BBBBATOM	4113	CG	PRO	B	203	12.593	-25.178	-3.084	1.00	24.04
BBBBATOM	4114	C	PRO	B	203	15.987	-23.731	-2.573	1.00	24.07
BBBBATOM	4115	O	PRO	B	203	16.395	-22.593	-2.343	1.00	23.18
BBBBATOM	4116	N	GLN	B	204	16.706	-24.814	-2.290	1.00	25.26
BBBBATOM	4117	CA	GLN	B	204	18.033	-24.708	-1.684	1.00	26.34
BBBBATOM	4118	CB	GLN	B	204	18.474	-26.078	-1.157	1.00	28.67

BBBBATOM	4119	CG	GLN	B	204	17.555	-26.626	-0.065	1.00 33.65
BBBBATOM	4120	CD	GLN	B	204	17.885	-28.059	0.328	1.00 37.09
BBBBATOM	4121	OE1	GLN	B	204	18.991	-28.354	0.792	1.00 39.30
BBBBATOM	4122	NE2	GLN	B	204	16.924	-28.960	0.140	1.00 38.32
BBBBATOM	4123	C	GLN	B	204	19.030	-24.177	-2.717	1.00 25.36
BBBBATOM	4124	O	GLN	B	204	19.985	-23.466	-2.385	1.00 24.98
BBBBATOM	4125	N	VAL	B	205	18.806	-24.522	-3.978	1.00 24.46
BBBBATOM	4126	CA	VAL	B	205	19.672	-24.033	-5.043	1.00 24.44
BBBBATOM	4127	CB	VAL	B	205	19.288	-24.634	-6.409	1.00 24.84
BBBBATOM	4128	CG1	VAL	B	205	20.039	-23.906	-7.534	1.00 23.72
BBBBATOM	4129	CG2	VAL	B	205	19.614	-26.110	-6.428	1.00 22.91
BBBBATOM	4130	C	VAL	B	205	19.511	-22.515	-5.110	1.00 23.79
BBBBATOM	4131	O	VAL	B	205	20.487	-21.789	-5.270	1.00 25.25
BBBBATOM	4132	N	ALA	B	206	18.273	-22.044	-4.972	1.00 24.12
BBBBATOM	4133	CA	ALA	B	206	17.980	-20.610	-5.013	1.00 22.84
BBBBATOM	4134	CB	ALA	B	206	16.466	-20.377	-4.908	1.00 21.55
BBBBATOM	4135	C	ALA	B	206	18.700	-19.862	-3.890	1.00 24.09
BBBBATOM	4136	O	ALA	B	206	19.174	-18.740	-4.081	1.00 24.90
BBBBATOM	4137	N	ALA	B	207	18.768	-20.477	-2.713	1.00 25.15
BBBBATOM	4138	CA	ALA	B	207	19.442	-19.857	-1.576	1.00 26.65
BBBBATOM	4139	CB	ALA	B	207	19.260	-20.710	-0.324	1.00 27.83
BBBBATOM	4140	C	ALA	B	207	20.924	-19.686	-1.879	1.00 26.96
BBBBATOM	4141	O	ALA	B	207	21.537	-18.693	-1.493	1.00 27.82
BBBBATOM	4142	N	LYS	B	208	21.498	-20.651	-2.586	1.00 27.19
BBBBATOM	4143	CA	LYS	B	208	22.915	-20.595	-2.919	1.00 28.31
BBBBATOM	4144	CB	LYS	B	208	23.432	-21.989	-3.300	1.00 29.85
BBBBATOM	4145	CG	LYS	B	208	23.030	-23.088	-2.329	1.00 32.97
BBBBATOM	4146	CD	LYS	B	208	23.264	-22.667	-0.886	1.00 35.74
BBBBATOM	4147	CE	LYS	B	208	22.689	-23.689	0.084	1.00 37.28
BBBBATOM	4148	NZ	LYS	B	208	21.227	-23.899	-0.135	1.00 35.29
BBBBATOM	4149	C	LYS	B	208	23.237	-19.624	-4.050	1.00 27.83
BBBBATOM	4150	O	LYS	B	208	24.286	-18.978	-4.033	1.00 27.46
BBBBATOM	4151	N	LEU	B	209	22.341	-19.517	-5.028	1.00 26.04
BBBBATOM	4152	CA	LEU	B	209	22.577	-18.640	-6.171	1.00 25.68
BBBBATOM	4153	CB	LEU	B	209	21.975	-19.268	-7.435	1.00 25.08
BBBBATOM	4154	CG	LEU	B	209	22.534	-20.638	-7.844	1.00 25.01
BBBBATOM	4155	CD1	LEU	B	209	21.797	-21.151	-9.074	1.00 25.67
BBBBATOM	4156	CD2	LEU	B	209	24.029	-20.528	-8.119	1.00 25.13
BBBBATOM	4157	C	LEU	B	209	22.075	-17.200	-6.007	1.00 25.59
BBBBATOM	4158	O	LEU	B	209	22.496	-16.313	-6.742	1.00 25.26
BBBBATOM	4159	N	GLY	B	210	21.185	-16.970	-5.045	1.00 26.27
BBBBATOM	4160	CA	GLY	B	210	20.675	-15.628	-4.804	1.00 26.56
BBBBATOM	4161	C	GLY	B	210	20.238	-14.836	-6.030	1.00 27.75
BBBBATOM	4162	O	GLY	B	210	19.518	-15.349	-6.889	1.00 27.68
BBBBATOM	4163	N	ASP	B	211	20.696	-13.585	-6.105	1.00 27.93
BBBBATOM	4164	CA	ASP	B	211	20.370	-12.647	-7.190	1.00 28.28
BBBBATOM	4165	CB	ASP	B	211	21.011	-11.283	-6.906	1.00 29.89
BBBBATOM	4166	CG	ASP	B	211	20.351	-10.545	-5.768	1.00 31.43
BBBBATOM	4167	OD1	ASP	B	211	20.864	-9.469	-5.398	1.00 32.43
BBBBATOM	4168	OD2	ASP	B	211	19.323	-11.025	-5.249	1.00 33.41
BBBBATOM	4169	C	ASP	B	211	20.768	-13.035	-8.615	1.00 27.77
BBBBATOM	4170	O	ASP	B	211	20.320	-12.397	-9.578	1.00 26.32
BBBBATOM	4171	N	SER	B	212	21.616	-14.048	-8.753	1.00 25.75
BBBBATOM	4172	CA	SER	B	212	22.098	-14.474	-10.067	1.00 25.73
BBBBATOM	4173	CB	SER	B	212	23.331	-15.376	-9.904	1.00 26.63
BBBBATOM	4174	OG	SER	B	212	22.971	-16.596	-9.282	1.00 26.71
BBBBATOM	4175	C	SER	B	212	21.062	-15.185	-10.943	1.00 23.61
BBBBATOM	4176	O	SER	B	212	21.262	-15.334	-12.147	1.00 22.28
BBBBATOM	4177	N	VAL	B	213	19.969	-15.644	-10.344	1.00 23.16
BBBBATOM	4178	CA	VAL	B	213	18.925	-16.308	-11.116	1.00 20.76
BBBBATOM	4179	CB	VAL	B	213	18.952	-17.867	-10.989	1.00 21.69
BBBBATOM	4180	CG1	VAL	B	213	20.318	-18.423	-11.375	1.00 19.84
BBBBATOM	4181	CG2	VAL	B	213	18.564	-18.288	-9.576	1.00 20.36
BBBBATOM	4182	C	VAL	B	213	17.535	-15.871	-10.677	1.00 21.41
BBBBATOM	4183	O	VAL	B	213	17.328	-15.396	-9.554	1.00 20.58
BBBBATOM	4184	N	THR	B	214	16.593	-16.021	-11.595	1.00 19.82

BBBBATOM	4185	CA	THR	B	214	15.204	-15.726	-11.337	1.00	19.60
BBBBATOM	4186	CB	THR	B	214	14.718	-14.478	-12.126	1.00	21.35
BBBBATOM	4187	OG1	THR	B	214	13.323	-14.273	-11.870	1.00	21.93
BBBBATOM	4188	CG2	THR	B	214	14.983	-14.633	-13.622	1.00	19.52
BBBBATOM	4189	C	THR	B	214	14.543	-17.021	-11.791	1.00	20.24
BBBBATOM	4190	O	THR	B	214	14.803	-17.533	-12.893	1.00	18.70
BBBBATOM	4191	N	ILE	B	215	13.706	-17.569	-10.921	1.00	19.21
BBBBATOM	4192	CA	ILE	B	215	13.076	-18.850	-11.169	1.00	18.75
BBBBATOM	4193	CB	ILE	B	215	13.417	-19.828	-10.008	1.00	18.82
BBBBATOM	4194	CG2	ILE	B	215	12.690	-21.157	-10.194	1.00	19.53
BBBBATOM	4195	CG1	ILE	B	215	14.934	-20.030	-9.931	1.00	19.76
BBBBATOM	4196	CD1	ILE	B	215	15.421	-20.656	-8.600	1.00	19.40
BBBBATOM	4197	C	ILE	B	215	11.568	-18.837	-11.315	1.00	19.26
BBBBATOM	4198	O	ILE	B	215	10.874	-18.025	-10.699	1.00	18.28
BBBBATOM	4199	N	TRP	B	216	11.089	-19.737	-12.167	1.00	18.93
BBBBATOM	4200	CA	TRP	B	216	9.661	-19.973	-12.378	1.00	19.34
BBBBATOM	4201	CB	TRP	B	216	9.222	-19.631	-13.797	1.00	18.97
BBBBATOM	4202	CG	TRP	B	216	7.757	-19.897	-14.065	1.00	20.09
BBBBATOM	4203	CD2	TRP	B	216	7.015	-19.467	-15.211	1.00	19.61
BBBBATOM	4204	CE2	TRP	B	216	5.705	-19.988	-15.085	1.00	19.98
BBBBATOM	4205	CE3	TRP	B	216	7.329	-18.690	-16.333	1.00	19.39
BBBBATOM	4206	CD1	TRP	B	216	6.888	-20.639	-13.303	1.00	19.30
BBBBATOM	4207	NE1	TRP	B	216	5.653	-20.700	-13.914	1.00	20.95
BBBBATOM	4208	CZ2	TRP	B	216	4.713	-19.759	-16.043	1.00	22.06
BBBBATOM	4209	CZ3	TRP	B	216	6.336	-18.459	-17.288	1.00	20.42
BBBBATOM	4210	CH2	TRP	B	216	5.047	-18.993	-17.134	1.00	21.16
BBBBATOM	4211	C	TRP	B	216	9.629	-21.479	-12.176	1.00	19.95
BBBBATOM	4212	O	TRP	B	216	10.114	-22.241	-13.010	1.00	19.91
BBBBATOM	4213	N	HIS	B	217	9.067	-21.897	-11.050	1.00	21.62
BBBBATOM	4214	CA	HIS	B	217	9.015	-23.303	-10.680	1.00	21.06
BBBBATOM	4215	CB	HIS	B	217	9.553	-23.419	-9.242	1.00	20.56
BBBBATOM	4216	CG	HIS	B	217	9.717	-24.824	-8.747	1.00	21.95
BBBBATOM	4217	CD2	HIS	B	217	8.915	-25.910	-8.846	1.00	22.12
BBBBATOM	4218	ND1	HIS	B	217	10.807	-25.219	-8.002	1.00	23.39
BBBBATOM	4219	CE1	HIS	B	217	10.670	-26.490	-7.663	1.00	21.82
BBBBATOM	4220	NE2	HIS	B	217	9.530	-26.933	-8.162	1.00	22.14
BBBBATOM	4221	C	HIS	B	217	7.596	-23.870	-10.795	1.00	21.27
BBBBATOM	4222	O	HIS	B	217	6.655	-23.334	-10.214	1.00	21.69
BBBBATOM	4223	N	GLN	B	218	7.448	-24.940	-11.567	1.00	20.83
BBBBATOM	4224	CA	GLN	B	218	6.149	-25.594	-11.735	1.00	24.30
BBBBATOM	4225	CB	GLN	B	218	5.915	-25.935	-13.206	1.00	23.84
BBBBATOM	4226	CG	GLN	B	218	4.561	-26.558	-13.495	1.00	25.91
BBBBATOM	4227	CD	GLN	B	218	4.637	-28.060	-13.673	1.00	26.52
BBBBATOM	4228	OE1	GLN	B	218	3.757	-28.793	-13.214	1.00	28.05
BBBBATOM	4229	NE2	GLN	B	218	5.680	-28.529	-14.360	1.00	25.20
BBBBATOM	4230	C	GLN	B	218	6.173	-26.854	-10.854	1.00	24.64
BBBBATOM	4231	O	GLN	B	218	6.780	-27.866	-11.199	1.00	25.73
BBBBATOM	4232	N	SER	B	219	5.502	-26.756	-9.709	1.00	26.38
BBBBATOM	4233	CA	SER	B	219	5.463	-27.800	-8.684	1.00	26.73
BBBBATOM	4234	CB	SER	B	219	4.947	-27.188	-7.380	1.00	28.26
BBBBATOM	4235	OG	SER	B	219	3.563	-26.881	-7.488	1.00	26.22
BBBBATOM	4236	C	SER	B	219	4.689	-29.096	-8.914	1.00	27.58
BBBBATOM	4237	O	SER	B	219	5.014	-30.122	-8.320	1.00	26.39
BBBBATOM	4238	N	GLY	B	220	3.662	-29.054	-9.750	1.00	28.58
BBBBATOM	4239	CA	GLY	B	220	2.855	-30.242	-9.961	1.00	30.53
BBBBATOM	4240	C	GLY	B	220	1.596	-30.110	-9.111	1.00	31.96
BBBBATOM	4241	O	GLY	B	220	1.523	-29.248	-8.233	1.00	30.92
BBBBATOM	4242	N	LYS	B	221	0.608	-30.965	-9.358	1.00	33.93
BBBBATOM	4243	CA	LYS	B	221	-0.657	-30.914	-8.628	1.00	35.12
BBBBATOM	4244	CB	LYS	B	221	-1.573	-32.049	-9.094	1.00	37.88
BBBBATOM	4245	CG	LYS	B	221	-2.942	-32.055	-8.427	1.00	40.51
BBBBATOM	4246	CD	LYS	B	221	-3.792	-33.215	-8.934	1.00	42.62
BBBBATOM	4247	CE	LYS	B	221	-5.162	-33.249	-8.260	1.00	43.67
BBBBATOM	4248	NZ	LYS	B	221	-6.002	-34.383	-8.763	1.00	45.38
BBBBATOM	4249	C	LYS	B	221	-0.545	-30.950	-7.103	1.00	35.13
BBBBATOM	4250	O	LYS	B	221	0.110	-31.823	-6.531	1.00	34.60

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BBBBATOM   4251  N   GLY B 222     -1.187 -29.979  -6.461  1.00 34.79
BBBBATOM   4252  CA  GLY B 222     -1.195 -29.899  -5.011  1.00 35.34
BBBBATOM   4253  C   GLY B 222      0.111 -29.594  -4.299  1.00 35.61
BBBBATOM   4254  O   GLY B 222      0.163 -29.678  -3.071  1.00 35.51
BBBBATOM   4255  N   SER B 223      1.158 -29.234  -5.038  1.00 34.65
BBBBATOM   4256  CA  SER B 223      2.451 -28.934  -4.418  1.00 33.98
BBBBATOM   4257  CB  SER B 223      3.552 -29.781  -5.062  1.00 35.02
BBBBATOM   4258  OG  SER B 223      3.303 -31.168  -4.897  1.00 36.07
BBBBATOM   4259  C   SER B 223      2.839 -27.454  -4.504  1.00 33.55
BBBBATOM   4260  O   SER B 223      3.930 -27.063  -4.086  1.00 31.72
BBBBATOM   4261  N   GLN B 224      1.941 -26.639  -5.044  1.00 33.22
BBBBATOM   4262  CA  GLN B 224      2.187 -25.208  -5.186  1.00 33.71
BBBBATOM   4263  CB  GLN B 224      0.954 -24.539  -5.799  1.00 35.45
BBBBATOM   4264  CG  GLN B 224      1.160 -23.120  -6.337  1.00 37.82
BBBBATOM   4265  CD  GLN B 224      1.344 -22.076  -5.249  1.00 40.08
BBBBATOM   4266  OE1 GLN B 224      0.669 -22.111  -4.217  1.00 40.97
BBBBATOM   4267  NE2 GLN B 224      2.244 -21.124  -5.486  1.00 40.08
BBBBATOM   4268  C   GLN B 224      2.510 -24.560  -3.840  1.00 33.86
BBBBATOM   4269  O   GLN B 224      3.512 -23.856  -3.697  1.00 33.38
BBBBATOM   4270  N   GLN B 225      1.659 -24.814  -2.850  1.00 33.06
BBBBATOM   4271  CA  GLN B 225      1.823 -24.239  -1.519  1.00 32.32
BBBBATOM   4272  CB  GLN B 225      0.624 -24.619  -0.640  1.00 35.12
BBBBATOM   4273  CG  GLN B 225     -0.743 -24.143  -1.151  1.00 36.85
BBBBATOM   4274  CD  GLN B 225     -1.144 -24.751  -2.495  1.00 39.09
BBBBATOM   4275  OE1 GLN B 225     -0.914 -25.937  -2.759  1.00 39.42
BBBBATOM   4276  NE2 GLN B 225     -1.768 -23.937  -3.345  1.00 40.13
BBBBATOM   4277  C   GLN B 225      3.117 -24.606  -0.788  1.00 30.73
BBBBATOM   4278  O   GLN B 225      3.766 -23.742  -0.202  1.00 30.36
BBBBATOM   4279  N   SER B 226      3.494 -25.878  -0.817  1.00 29.26
BBBBATOM   4280  CA  SER B 226      4.701 -26.309  -0.122  1.00 28.30
BBBBATOM   4281  CB  SER B 226      4.727 -27.834   0.003  1.00 29.10
BBBBATOM   4282  OG  SER B 226      4.563 -28.461  -1.254  1.00 32.61
BBBBATOM   4283  C   SER B 226      5.991 -25.809  -0.771  1.00 26.41
BBBBATOM   4284  O   SER B 226      6.950 -25.486  -0.073  1.00 25.24
BBBBATOM   4285  N   VAL B 227      6.019 -25.738  -2.099  1.00 25.21
BBBBATOM   4286  CA  VAL B 227      7.214 -25.247  -2.791  1.00 24.28
BBBBATOM   4287  CB  VAL B 227      7.150 -25.527  -4.317  1.00 23.32
BBBBATOM   4288  CG1 VAL B 227      8.368 -24.914  -5.028  1.00 20.67
BBBBATOM   4289  CG2 VAL B 227      7.117 -27.024  -4.563  1.00 22.45
BBBBATOM   4290  C   VAL B 227      7.335 -23.743  -2.545  1.00 24.34
BBBBATOM   4291  O   VAL B 227      8.421 -23.240  -2.281  1.00 25.50
BBBBATOM   4292  N   GLU B 228      6.209 -23.035  -2.623  1.00 26.12
BBBBATOM   4293  CA  GLU B 228      6.178 -21.592  -2.387  1.00 27.23
BBBBATOM   4294  CB  GLU B 228      4.735 -21.075  -2.476  1.00 28.60
BBBBATOM   4295  CG  GLU B 228      4.558 -19.586  -2.184  1.00 30.24
BBBBATOM   4296  CD  GLU B 228      4.938 -18.688  -3.356  1.00 31.99
BBBBATOM   4297  OE1 GLU B 228      5.012 -17.452  -3.159  1.00 31.68
BBBBATOM   4298  OE2 GLU B 228      5.154 -19.212  -4.471  1.00 32.04
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BBBBATOM   4301  N   GLN B 229      6.374 -22.178  -0.041  1.00 28.66
BBBBATOM   4302  CA  GLN B 229      6.853 -22.046   1.329  1.00 28.39
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BBBBATOM   4306  OE1 GLN B 229      4.548 -23.810   4.645  1.00 39.26
BBBBATOM   4307  NE2 GLN B 229      6.484 -24.697   5.370  1.00 38.61
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BBBBATOM   4310  N   ALA B 230      8.771 -23.385   0.677  1.00 26.97
BBBBATOM   4311  CA  ALA B 230     10.185 -23.754   0.682  1.00 26.18
BBBBATOM   4312  CB  ALA B 230     10.412 -24.984  -0.184  1.00 25.07
BBBBATOM   4313  C   ALA B 230     11.054 -22.588   0.192  1.00 26.36
BBBBATOM   4314  O   ALA B 230     12.119 -22.317   0.755  1.00 25.04
BBBBATOM   4315  N   TYR B 231     10.605 -21.895  -0.854  1.00 25.85
BBBBATOM   4316  CA  TYR B 231     11.371 -20.766  -1.366  1.00 25.47
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BBBBATOM   4317  CB  TYR B 231      10.762 -20.248  -2.678  1.00 24.72
BBBBATOM   4318  CG  TYR B 231      11.236 -21.014  -3.905  1.00 23.66
BBBBATOM   4319  CD1 TYR B 231      12.546 -20.869  -4.381  1.00 23.97
BBBBATOM   4320  CE1 TYR B 231      13.006 -21.599  -5.488  1.00 21.40
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BBBBATOM   4322  CE2 TYR B 231      10.841 -22.641  -5.681  1.00 22.71
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BBBBATOM   4324  OH  TYR B 231      12.600 -23.214  -7.199  1.00 21.69
BBBBATOM   4325  C   TYR B 231      11.450 -19.639  -0.336  1.00 26.53
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BBBBATOM   4342  CA  ALA B 234      15.215 -20.417   1.714  1.00 28.48
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BBBBATOM   4362  CB  PRO B 237       9.808 -14.798  -0.527  1.00 25.37
BBBBATOM   4363  CG  PRO B 237      10.862 -13.773  -0.340  1.00 25.24
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BBBBATOM   4369  CG  GLN B 238      12.622 -12.945  -5.852  1.00 25.22
BBBBATOM   4370  CD  GLN B 238      13.535 -13.523  -4.783  1.00 26.90
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BBBBATOM   4380  ND1 HIS B 239      13.488 -16.743  -7.992  1.00 20.30
BBBBATOM   4381  CE1 HIS B 239      14.769 -16.582  -7.711  1.00 22.38
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BBBBATOM	4423	CE1	PHE	B	244	-1.335	-29.744	-12.328	1.00	33.63
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BBBBATOM   4481  CD2 TYR B 252      10.288 -24.505 -22.319  1.00 22.30
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BBBBATOM   4484  OH  TYR B 252       9.554 -28.088 -22.305  1.00 25.57
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BBBBATOM   4492  N   TRP B 254      10.299 -17.369 -22.379  1.00 20.49
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BBBBATOM   4502  CZ3 TRP B 254      11.504 -18.642 -16.346  1.00 20.05
BBBBATOM   4503  CH2 TRP B 254      11.991 -17.743 -15.380  1.00 18.31
BBBBATOM   4504  C   TRP B 254      12.156 -17.059 -20.755  1.00 19.33
BBBBATOM   4505  O   TRP B 254      13.084 -16.293 -20.496  1.00 19.25
BBBBATOM   4506  N   ALA B 255      12.234 -18.373 -20.597  1.00 18.90
BBBBATOM   4507  CA  ALA B 255      13.399 -19.025 -20.003  1.00 19.51
BBBBATOM   4508  CB  ALA B 255      13.082 -20.507 -19.788  1.00 18.83
BBBBATOM   4509  C   ALA B 255      14.737 -18.901 -20.713  1.00 18.88
BBBBATOM   4510  O   ALA B 255      14.803 -18.688 -21.918  1.00 19.40
BBBBATOM   4511  N   ASP B 256      15.803 -19.036 -19.927  1.00 19.01
BBBBATOM   4512  CA  ASP B 256      17.176 -19.026 -20.434  1.00 17.58
BBBBATOM   4513  CB  ASP B 256      18.078 -18.185 -19.534  1.00 18.47
BBBBATOM   4514  CG  ASP B 256      17.954 -16.699 -19.795  1.00 18.05
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BBBBATOM	4515	OD1	ASP	B	256	17.845	-15.944	-18.806	1.00 16.89
BBBBATOM	4516	OD2	ASP	B	256	17.983	-16.287	-20.982	1.00 19.53
BBBBATOM	4517	C	ASP	B	256	17.657	-20.481	-20.379	1.00 18.01
BBBBATOM	4518	O	ASP	B	256	18.459	-20.929	-21.198	1.00 16.11
BBBBATOM	4519	N	VAL	B	257	17.147	-21.216	-19.396	1.00 17.49
BBBBATOM	4520	CA	VAL	B	257	17.535	-22.603	-19.194	1.00 18.53
BBBBATOM	4521	CB	VAL	B	257	18.831	-22.681	-18.332	1.00 17.72
BBBBATOM	4522	CG1	VAL	B	257	18.586	-22.069	-16.966	1.00 19.19
BBBBATOM	4523	CG2	VAL	B	257	19.286	-24.129	-18.200	1.00 20.40
BBBBATOM	4524	C	VAL	B	257	16.400	-23.363	-18.501	1.00 18.31
BBBBATOM	4525	O	VAL	B	257	15.659	-22.795	-17.703	1.00 19.74
BBBBATOM	4526	N	VAL	B	258	16.263	-24.643	-18.818	1.00 18.74
BBBBATOM	4527	CA	VAL	B	258	15.208	-25.456	-18.234	1.00 19.32
BBBBATOM	4528	CB	VAL	B	258	14.328	-26.100	-19.337	1.00 19.89
BBBBATOM	4529	CG1	VAL	B	258	13.101	-26.754	-18.714	1.00 19.81
BBBBATOM	4530	CG2	VAL	B	258	13.907	-25.041	-20.364	1.00 21.59
BBBBATOM	4531	C	VAL	B	258	15.799	-26.585	-17.389	1.00 19.70
BBBBATOM	4532	O	VAL	B	258	16.808	-27.175	-17.758	1.00 18.96
BBBBATOM	4533	N	VAL	B	259	15.167	-26.861	-16.253	1.00 20.24
BBBBATOM	4534	CA	VAL	B	259	15.581	-27.957	-15.374	1.00 19.85
BBBBATOM	4535	CB	VAL	B	259	15.850	-27.483	-13.936	1.00 20.08
BBBBATOM	4536	CG1	VAL	B	259	16.222	-28.689	-13.059	1.00 20.22
BBBBATOM	4537	CG2	VAL	B	259	16.966	-26.453	-13.930	1.00 17.86
BBBBATOM	4538	C	VAL	B	259	14.382	-28.890	-15.371	1.00 20.02
BBBBATOM	4539	O	VAL	B	259	13.301	-28.500	-14.942	1.00 21.88
BBBBATOM	4540	N	CYS	B	260	14.562	-30.111	-15.867	1.00 21.70
BBBBATOM	4541	CA	CYS	B	260	13.454	-31.055	-15.946	1.00 22.00
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BBBBATOM	4544	C	CYS	B	260	13.903	-32.478	-16.242	1.00 21.86
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BBBBATOM	4547	CA	ARG	B	261	13.170	-34.800	-16.515	1.00 23.75
BBBBATOM	4548	CB	ARG	B	261	11.964	-35.663	-16.104	1.00 27.16
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BBBBATOM	4550	CD	ARG	B	261	11.490	-36.473	-13.732	1.00 36.33
BBBBATOM	4551	NE	ARG	B	261	12.865	-36.721	-13.323	1.00 38.48
BBBBATOM	4552	CZ	ARG	B	261	13.218	-37.176	-12.125	1.00 37.25
BBBBATOM	4553	NH1	ARG	B	261	12.295	-37.433	-11.204	1.00 38.46
BBBBATOM	4554	NH2	ARG	B	261	14.499	-37.370	-11.848	1.00 36.79
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BBBBATOM	4556	O	ARG	B	261	13.117	-33.883	-18.746	1.00 22.44
BBBBATOM	4557	N	SER	B	262	13.740	-36.038	-18.527	1.00 22.00
BBBBATOM	4558	CA	SER	B	262	13.975	-36.189	-19.948	1.00 23.18
BBBBATOM	4559	CB	SER	B	262	15.481	-36.377	-20.203	1.00 24.45
BBBBATOM	4560	OG	SER	B	262	16.043	-37.326	-19.311	1.00 25.79
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BBBBATOM	4563	N	GLY	B	263	11.850	-37.151	-20.619	1.00 22.74
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BBBBATOM	4567	N	ALA	B	264	11.130	-38.739	-23.708	1.00 23.37
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BBBBATOM	4573	CA	LEU	B	265	8.846	-36.037	-26.205	1.00 24.66
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BBBBATOM	4575	CG	LEU	B	265	6.760	-37.544	-26.426	1.00 27.97
BBBBATOM	4576	CD1	LEU	B	265	5.242	-37.541	-26.258	1.00 28.21
BBBBATOM	4577	CD2	LEU	B	265	7.146	-37.856	-27.878	1.00 27.40
BBBBATOM	4578	C	LEU	B	265	9.331	-34.717	-25.613	1.00 24.47
BBBBATOM	4579	O	LEU	B	265	9.374	-33.693	-26.301	1.00 23.85
BBBBATOM	4580	N	THR	B	266	9.702	-34.747	-24.338	1.00 22.12

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BBBBATOM   4581  CA  THR B 266      10.194 -33.557 -23.657  1.00 22.34
BBBBATOM   4582  CB  THR B 266      10.348 -33.803 -22.140  1.00 22.35
BBBBATOM   4583  OG1 THR B 266       9.061 -34.087 -21.583  1.00 24.46
BBBBATOM   4584  CG2 THR B 266      10.945 -32.573 -21.444  1.00 24.00
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BBBBATOM   4586  O   THR B 266      11.761 -31.926 -24.442  1.00 20.35
BBBBATOM   4587  N   VAL B 267      12.427 -34.075 -24.461  1.00 20.46
BBBBATOM   4588  CA  VAL B 267      13.730 -33.762 -25.023  1.00 21.11
BBBBATOM   4589  CB  VAL B 267      14.614 -35.039 -25.114  1.00 21.54
BBBBATOM   4590  CG1 VAL B 267      15.903 -34.740 -25.865  1.00 20.72
BBBBATOM   4591  CG2 VAL B 267      14.938 -35.541 -23.708  1.00 20.45
BBBBATOM   4592  C   VAL B 267      13.548 -33.138 -26.416  1.00 21.34
BBBBATOM   4593  O   VAL B 267      14.188 -32.135 -26.747  1.00 19.99
BBBBATOM   4594  N   SER B 268      12.663 -33.717 -27.222  1.00 21.61
BBBBATOM   4595  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96
BBBBATOM   4596  CB  SER B 268      11.474 -34.121 -29.344  1.00 21.57
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BBBBATOM   4598  C   SER B 268      11.817 -31.790 -28.519  1.00 21.81
BBBBATOM   4599  O   SER B 268      12.158 -30.933 -29.336  1.00 22.60
BBBBATOM   4600  N   GLU B 269      10.928 -31.563 -27.557  1.00 21.64
BBBBATOM   4601  CA  GLU B 269      10.282 -30.272 -27.378  1.00 21.95
BBBBATOM   4602  CB  GLU B 269       9.213 -30.399 -26.292  1.00 24.72
BBBBATOM   4603  CG  GLU B 269       8.480 -29.128 -25.940  1.00 27.67
BBBBATOM   4604  CD  GLU B 269       7.385 -29.380 -24.908  1.00 30.05
BBBBATOM   4605  OE1 GLU B 269       6.325 -29.915 -25.287  1.00 31.50
BBBBATOM   4606  OE2 GLU B 269       7.591 -29.057 -23.719  1.00 29.84
BBBBATOM   4607  C   GLU B 269      11.321 -29.214 -26.999  1.00 21.68
BBBBATOM   4608  O   GLU B 269      11.301 -28.095 -27.518  1.00 18.12
BBBBATOM   4609  N   ILE B 270      12.224 -29.581 -26.092  1.00 19.43
BBBBATOM   4610  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62
BBBBATOM   4611  CB  ILE B 270      14.157 -29.391 -24.533  1.00 20.30
BBBBATOM   4612  CG2 ILE B 270      15.415 -28.595 -24.266  1.00 19.17
BBBBATOM   4613  CG1 ILE B 270      13.337 -29.574 -23.254  1.00 21.32
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BBBBATOM   4615  C   ILE B 270      14.214 -28.314 -26.806  1.00 20.58
BBBBATOM   4616  O   ILE B 270      14.595 -27.151 -26.954  1.00 20.50
BBBBATOM   4617  N   ALA B 271      14.574 -29.298 -27.624  1.00 21.29
BBBBATOM   4618  CA  ALA B 271      15.440 -29.058 -28.776  1.00 22.45
BBBBATOM   4619  CB  ALA B 271      15.741 -30.376 -29.485  1.00 23.36
BBBBATOM   4620  C   ALA B 271      14.766 -28.084 -29.745  1.00 23.03
BBBBATOM   4621  O   ALA B 271      15.400 -27.156 -30.259  1.00 23.57
BBBBATOM   4622  N   ALA B 272      13.479 -28.301 -29.988  1.00 21.81
BBBBATOM   4623  CA  ALA B 272      12.719 -27.451 -30.898  1.00 22.17
BBBBATOM   4624  CB  ALA B 272      11.335 -28.053 -31.131  1.00 22.15
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BBBBATOM   4626  O   ALA B 272      12.585 -25.058 -31.122  1.00 21.77
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BBBBATOM   4631  O   ALA B 273      13.754 -22.642 -28.344  1.00 22.67
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BBBBATOM   4633  CA  GLY B 274      16.093 -24.023 -28.709  1.00 21.07
BBBBATOM   4634  C   GLY B 274      16.498 -23.549 -27.327  1.00 21.48
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BBBBATOM   4637  CA  LEU B 275      16.666 -24.057 -24.966  1.00 19.78
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BBBBATOM   4639  CG  LEU B 275      14.451 -22.870 -24.202  1.00 24.60
BBBBATOM   4640  CD1 LEU B 275      13.220 -23.136 -23.349  1.00 26.44
BBBBATOM   4641  CD2 LEU B 275      15.159 -21.609 -23.725  1.00 24.02
BBBBATOM   4642  C   LEU B 275      17.698 -24.970 -24.318  1.00 18.79
BBBBATOM   4643  O   LEU B 275      17.679 -26.180 -24.524  1.00 19.36
BBBBATOM   4644  N   PRO B 276      18.634 -24.389 -23.554  1.00 17.27
BBBBATOM   4645  CD  PRO B 276      18.925 -22.955 -23.416  1.00 16.95
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BBBBATOM	4665	CA	PHE	B	279	18.266	-32.838	-17.392	1.00	21.59
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BBBBATOM	4667	CG	PHE	B	279	17.740	-33.099	-19.876	1.00	19.35
BBBBATOM	4668	CD1	PHE	B	279	18.481	-32.898	-21.035	1.00	19.42
BBBBATOM	4669	CD2	PHE	B	279	16.379	-32.794	-19.888	1.00	18.16
BBBBATOM	4670	CE1	PHE	B	279	17.874	-32.405	-22.203	1.00	19.06
BBBBATOM	4671	CE2	PHE	B	279	15.759	-32.298	-21.052	1.00	17.65
BBBBATOM	4672	CZ	PHE	B	279	16.515	-32.108	-22.208	1.00	15.61
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BBBBATOM	4676	CA	VAL	B	280	17.502	-34.902	-14.281	1.00	25.67
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BBBBATOM	4682	N	PRO	B	281	17.324	-37.080	-15.370	1.00	27.09
BBBBATOM	4683	CD	PRO	B	281	18.750	-37.057	-15.726	1.00	27.31
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BBBBATOM	4689	N	PHE	B	282	14.908	-39.668	-14.923	1.00	33.83
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BBBBATOM	4691	CB	PHE	B	282	12.818	-40.808	-14.372	1.00	38.38
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BBBBATOM	4697	CZ	PHE	B	282	10.536	-43.085	-11.532	1.00	41.74
BBBBATOM	4698	C	PHE	B	282	15.078	-41.776	-13.880	1.00	38.09
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BBBBATOM	4700	N	GLN	B	283	15.492	-42.197	-12.690	1.00	39.70
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BBBBATOM	4705	OE1	GLN	B	283	20.199	-44.068	-11.712	1.00	43.66
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BBBBATOM	4710	CA	HIS	B	284	15.641	-46.917	-13.843	1.00	43.69
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BBBBATOM	4712	CG	HIS	B	284	13.795	-48.039	-15.165	1.00	44.71

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BBBBATOM   4713  CD2 HIS B 284      12.574 -48.489 -14.793  1.00 44.80
BBBBATOM   4714  ND1 HIS B 284      14.360 -49.044 -15.923  1.00 44.69
BBBBATOM   4715  CE1 HIS B 284      13.516 -50.058 -16.002  1.00 45.06
BBBBATOM   4716  NE2 HIS B 284      12.425 -49.747 -15.325  1.00 44.90
BBBBATOM   4717  C   HIS B 284      16.749 -47.788 -14.424  1.00 44.09
BBBBATOM   4718  O   HIS B 284      17.602 -47.302 -15.164  1.00 43.02
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BBBBATOM   4946  CB  ASP B 313      26.840 -28.656  -4.120  1.00 32.36
BBBBATOM   4947  CG  ASP B 313      26.817 -28.085  -2.718  1.00 34.21
BBBBATOM   4948  OD1 ASP B 313      26.662 -26.855  -2.578  1.00 36.52
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BBBBATOM   4950  C   ASP B 313      25.910 -28.516  -6.425  1.00 28.84
BBBBATOM   4951  O   ASP B 313      26.442 -27.677  -7.146  1.00 28.96
BBBBATOM   4952  N   ALA B 314      25.555 -29.719  -6.868  1.00 26.61
BBBBATOM   4953  CA  ALA B 314      25.782 -30.099  -8.254  1.00 26.47
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BBBBATOM   4957  N   VAL B 315      23.661 -29.046  -8.815  1.00 25.00
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BBBBATOM   4960  CG1 VAL B 315      20.392 -27.382  -9.898  1.00 23.53
BBBBATOM   4961  CG2 VAL B 315      20.810 -29.738  -9.172  1.00 25.69
BBBBATOM   4962  C   VAL B 315      23.222 -26.764  -9.561  1.00 25.02
BBBBATOM   4963  O   VAL B 315      23.398 -26.125 -10.590  1.00 25.73
BBBBATOM   4964  N   ALA B 316      23.445 -26.251  -8.359  1.00 26.04
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BBBBATOM   4969  N   ASN B 317      26.178 -25.463  -8.823  1.00 28.72
BBBBATOM   4970  CA  ASN B 317      27.444 -25.246  -9.518  1.00 28.52
BBBBATOM   4971  CB  ASN B 317      28.493 -26.271  -9.081  1.00 31.30
BBBBATOM   4972  CG  ASN B 317      28.940 -26.068  -7.645  1.00 34.01
BBBBATOM   4973  OD1 ASN B 317      29.091 -24.933  -7.183  1.00 33.87
BBBBATOM   4974  ND2 ASN B 317      29.170 -27.171  -6.933  1.00 35.63
BBBBATOM   4975  C   ASN B 317      27.270 -25.310 -11.026  1.00 27.23
BBBBATOM   4976  O   ASN B 317      27.887 -24.543 -11.765  1.00 26.36
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BBBBATOM   4979  CB  THR B 318      25.203 -27.537 -13.189  1.00 27.91
BBBBATOM   4980  OG1 THR B 318      25.843 -28.779 -12.872  1.00 30.24
BBBBATOM   4981  CG2 THR B 318      24.784 -27.539 -14.655  1.00 27.49
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BBBBATOM   4984  N   LEU B 319      24.516 -24.588 -12.859  1.00 24.75
BBBBATOM   4985  CA  LEU B 319      23.883 -23.370 -13.357  1.00 25.21
BBBBATOM   4986  CB  LEU B 319      22.579 -23.090 -12.600  1.00 23.70
BBBBATOM   4987  CG  LEU B 319      21.496 -24.153 -12.803  1.00 23.20
BBBBATOM   4988  CD1 LEU B 319      20.384 -23.962 -11.785  1.00 22.93
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BBBBATOM   4991  O   LEU B 319      24.888 -21.368 -14.168  1.00 25.17
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BBBBATOM   4993  CA  ALA B 320      26.445 -20.931 -11.957  1.00 24.59
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BBBBATOM   5003  CB  TRP B 322      25.499 -21.841 -17.858  1.00 20.09
BBBBATOM   5004  CG  TRP B 322      25.763 -23.318 -17.973  1.00 19.85
BBBBATOM   5005  CD2 TRP B 322      24.789 -24.370 -17.939  1.00 19.16
BBBBATOM   5006  CE2 TRP B 322      25.479 -25.584 -18.164  1.00 20.31
BBBBATOM   5007  CE3 TRP B 322      23.403 -24.406 -17.742  1.00 19.35
BBBBATOM   5008  CD1 TRP B 322      26.973 -23.925 -18.204  1.00 19.51
BBBBATOM   5009  NE1 TRP B 322      26.806 -25.281 -18.323  1.00 18.84
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BBBBATOM   5014  O   TRP B 322      25.390 -19.030 -17.271  1.00 21.25
BBBBATOM   5015  N   SER B 323      27.320 -18.824 -18.409  1.00 19.53
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BBBBATOM   5027  CZ  ARG B 324      20.268 -13.403 -19.510  1.00 21.63
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BBBBATOM   5030  C   ARG B 324      25.288 -16.145 -22.481  1.00 17.79
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BBBBATOM   5037  OE1 GLU B 325      31.446 -16.562 -26.433  1.00 18.89
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BBBBATOM   5147  CB  PRO B 340      10.994 -28.349 -37.194  1.00 35.58
BBBBATOM   5148  CG  PRO B 340      12.052 -28.642 -38.205  1.00 36.27
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BBBBATOM   5154  CG  ASP B 341      10.101 -31.886 -41.159  1.00 37.02
BBBBATOM   5155  OD1 ASP B 341      11.125 -31.907 -40.443  1.00 37.17
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BBBBATOM   5157  C   ASP B 341       8.655 -33.336 -38.899  1.00 32.11
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BBBBATOM   5165  CA  THR B 343       5.115 -35.696 -37.744  1.00 28.55
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BBBBATOM   5167  OG1 THR B 343       4.119 -34.642 -35.782  1.00 28.04
BBBBATOM   5168  CG2 THR B 343       2.628 -35.330 -37.528  1.00 28.54
BBBBATOM   5169  C   THR B 343       4.934 -35.882 -39.254  1.00 29.50
BBBBATOM   5170  O   THR B 343       4.533 -36.952 -39.711  1.00 28.08
BBBBATOM   5171  N   GLU B 344       5.234 -34.843 -40.030  1.00 30.76
BBBBATOM   5172  CA  GLU B 344       5.085 -34.933 -41.480  1.00 32.00
BBBBATOM   5173  CB  GLU B 344       5.414 -33.589 -42.142  1.00 34.02
BBBBATOM   5174  CG  GLU B 344       4.412 -32.483 -41.814  1.00 38.27
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BBBBATOM	5175	CD	GLU	B	344	4.807	-31.661	-40.594	1.00	40.96
BBBBATOM	5176	OE1	GLU	B	344	5.252	-32.252	-39.582	1.00	41.33
BBBBATOM	5177	OE2	GLU	B	344	4.665	-30.419	-40.649	1.00	42.30
BBBBATOM	5178	C	GLU	B	344	5.970	-36.032	-42.056	1.00	31.14
BBBBATOM	5179	O	GLU	B	344	5.534	-36.805	-42.909	1.00	32.33
BBBBATOM	5180	N	ARG	B	345	7.209	-36.106	-41.587	1.00	30.66
BBBBATOM	5181	CA	ARG	B	345	8.138	-37.123	-42.067	1.00	31.44
BBBBATOM	5182	CB	ARG	B	345	9.494	-36.986	-41.376	1.00	33.54
BBBBATOM	5183	CG	ARG	B	345	10.293	-35.772	-41.793	1.00	37.73
BBBBATOM	5184	CD	ARG	B	345	11.716	-35.880	-41.284	1.00	40.70
BBBBATOM	5185	NE	ARG	B	345	12.580	-34.864	-41.873	1.00	44.36
BBBBATOM	5186	CZ	ARG	B	345	13.901	-34.841	-41.739	1.00	45.65
BBBBATOM	5187	NH1	ARG	B	345	14.514	-35.782	-41.031	1.00	46.05
BBBBATOM	5188	NH2	ARG	B	345	14.608	-33.881	-42.322	1.00	47.38
BBBBATOM	5189	C	ARG	B	345	7.626	-38.545	-41.854	1.00	30.89
BBBBATOM	5190	O	ARG	B	345	7.724	-39.387	-42.746	1.00	29.98
BBBBATOM	5191	N	VAL	B	346	7.086	-38.818	-40.670	1.00	29.72
BBBBATOM	5192	CA	VAL	B	346	6.578	-40.151	-40.384	1.00	28.61
BBBBATOM	5193	CB	VAL	B	346	6.197	-40.298	-38.885	1.00	27.90
BBBBATOM	5194	CG1	VAL	B	346	5.612	-41.680	-38.625	1.00	27.30
BBBBATOM	5195	CG2	VAL	B	346	7.419	-40.060	-38.024	1.00	27.32
BBBBATOM	5196	C	VAL	B	346	5.361	-40.435	-41.252	1.00	28.33
BBBBATOM	5197	O	VAL	B	346	5.248	-41.511	-41.847	1.00	28.30
BBBBATOM	5198	N	ALA	B	347	4.457	-39.465	-41.335	1.00	28.76
BBBBATOM	5199	CA	ALA	B	347	3.249	-39.617	-42.137	1.00	28.96
BBBBATOM	5200	CB	ALA	B	347	2.363	-38.387	-41.994	1.00	28.49
BBBBATOM	5201	C	ALA	B	347	3.596	-39.844	-43.606	1.00	30.26
BBBBATOM	5202	O	ALA	B	347	2.948	-40.641	-44.279	1.00	30.12
BBBBATOM	5203	N	ASN	B	348	4.613	-39.142	-44.098	1.00	32.77
BBBBATOM	5204	CA	ASN	B	348	5.035	-39.286	-45.493	1.00	34.56
BBBBATOM	5205	CB	ASN	B	348	6.045	-38.195	-45.868	1.00	35.68
BBBBATOM	5206	CG	ASN	B	348	5.384	-36.846	-46.123	1.00	37.21
BBBBATOM	5207	OD1	ASN	B	348	4.157	-36.719	-46.081	1.00	38.48
BBBBATOM	5208	ND2	ASN	B	348	6.199	-35.831	-46.393	1.00	38.38
BBBBATOM	5209	C	ASN	B	348	5.633	-40.668	-45.765	1.00	34.90
BBBBATOM	5210	O	ASN	B	348	5.433	-41.233	-46.841	1.00	34.59
BBBBATOM	5211	N	GLU	B	349	6.366	-41.212	-44.794	1.00	35.20
BBBBATOM	5212	CA	GLU	B	349	6.954	-42.540	-44.956	1.00	34.86
BBBBATOM	5213	CB	GLU	B	349	8.004	-42.814	-43.879	1.00	34.59
BBBBATOM	5214	CG	GLU	B	349	9.404	-42.385	-44.259	1.00	38.16
BBBBATOM	5215	CD	GLU	B	349	9.865	-42.992	-45.579	1.00	38.74
BBBBATOM	5216	OE1	GLU	B	349	9.806	-44.232	-45.735	1.00	40.12
BBBBATOM	5217	OE2	GLU	B	349	10.292	-42.225	-46.461	1.00	39.64
BBBBATOM	5218	C	GLU	B	349	5.872	-43.607	-44.895	1.00	33.96
BBBBATOM	5219	O	GLU	B	349	5.942	-44.621	-45.591	1.00	33.99
BBBBATOM	5220	N	VAL	B	350	4.875	-43.377	-44.051	1.00	33.91
BBBBATOM	5221	CA	VAL	B	350	3.767	-44.306	-43.919	1.00	33.79
BBBBATOM	5222	CB	VAL	B	350	2.848	-43.907	-42.744	1.00	33.70
BBBBATOM	5223	CG1	VAL	B	350	1.554	-44.695	-42.798	1.00	32.22
BBBBATOM	5224	CG2	VAL	B	350	3.568	-44.154	-41.425	1.00	32.24
BBBBATOM	5225	C	VAL	B	350	2.969	-44.274	-45.217	1.00	34.78
BBBBATOM	5226	O	VAL	B	350	2.411	-45.285	-45.645	1.00	34.85
BBBBATOM	5227	N	SER	B	351	2.925	-43.102	-45.844	1.00	35.34
BBBBATOM	5228	CA	SER	B	351	2.196	-42.946	-47.095	1.00	36.67
BBBBATOM	5229	CB	SER	B	351	2.024	-41.462	-47.425	1.00	37.32
BBBBATOM	5230	OG	SER	B	351	1.241	-41.292	-48.590	1.00	37.74
BBBBATOM	5231	C	SER	B	351	2.958	-43.639	-48.222	1.00	37.35
BBBBATOM	5232	O	SER	B	351	2.365	-44.309	-49.064	1.00	36.85
BBBBATOM	5233	N	ARG	B	352	4.277	-43.482	-48.223	1.00	37.89
BBBBATOM	5234	CA	ARG	B	352	5.114	-44.088	-49.251	1.00	40.03
BBBBATOM	5235	CB	ARG	B	352	6.557	-43.600	-49.114	1.00	41.58
BBBBATOM	5236	CG	ARG	B	352	7.470	-44.069	-50.232	1.00	44.46
BBBBATOM	5237	CD	ARG	B	352	8.906	-44.157	-49.759	1.00	47.36
BBBBATOM	5238	NE	ARG	B	352	9.097	-45.271	-48.832	1.00	49.57
BBBBATOM	5239	CZ	ARG	B	352	10.234	-45.524	-48.191	1.00	50.54
BBBBATOM	5240	NH1	ARG	B	352	11.287	-44.738	-48.372	1.00	50.88

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BBBBATOM   5241  NH2 ARG B 352      10.321 -46.566 -47.373  1.00 50.24
BBBBATOM   5242  C   ARG B 352       5.098 -45.613 -49.176  1.00 40.60
BBBBATOM   5243  O   ARG B 352       5.101 -46.292 -50.204  1.00 39.84
BBBBATOM   5244  N   VAL B 353       5.096 -46.143 -47.955  1.00 41.33
BBBBATOM   5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78
BBBBATOM   5246  CB  VAL B 353       5.446 -47.927 -46.271  1.00 42.54
BBBBATOM   5247  CG1 VAL B 353       5.279 -49.420 -46.014  1.00 42.05
BBBBATOM   5248  CG2 VAL B 353       6.879 -47.509 -45.987  1.00 41.86
BBBBATOM   5249  C   VAL B 353       3.742 -48.206 -48.095  1.00 43.85
BBBBATOM   5250  O   VAL B 353       3.679 -49.343 -48.556  1.00 44.43
BBBBATOM   5251  N   ALA B 354       2.664 -47.465 -47.871  1.00 45.85
BBBBATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24
BBBBATOM   5253  CB  ALA B 354       0.264 -47.043 -47.628  1.00 46.79
BBBBATOM   5254  C   ALA B 354       1.250 -47.971 -49.737  1.00 48.54
BBBBATOM   5255  O   ALA B 354       0.531 -48.780 -50.324  1.00 48.48
BBBBATOM   5256  N   ARG B 355       1.998 -47.068 -50.366  1.00 50.49
BBBBATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71
BBBBATOM   5258  CB  ARG B 355       2.658 -45.633 -52.264  1.00 53.58
BBBBATOM   5259  CG  ARG B 355       1.998 -44.372 -51.730  1.00 55.08
BBBBATOM   5260  CD  ARG B 355       0.716 -44.014 -52.461  1.00 56.64
BBBBATOM   5261  NE  ARG B 355       0.112 -42.802 -51.907  1.00 57.43
BBBBATOM   5262  CZ  ARG B 355      -1.054 -42.296 -52.299  1.00 58.24
BBBBATOM   5263  NH1 ARG B 355      -1.758 -42.896 -53.252  1.00 58.53
BBBBATOM   5264  NH2 ARG B 355      -1.519 -41.186 -51.738  1.00 58.87
BBBBATOM   5265  C   ARG B 355       2.899 -48.099 -52.366  1.00 53.41
BBBBATOM   5266  O   ARG B 355       2.966 -48.319 -53.575  1.00 53.50
BBBBATOM   5267  N   ALA B 356       3.569 -48.805 -51.456  1.00 54.15
BBBBATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93
BBBBATOM   5269  CB  ALA B 356       3.669 -51.004 -52.546  1.00 54.86
BBBBATOM   5270  C   ALA B 356       5.611 -49.417 -52.671  1.00 55.63
BBBBATOM   5271  O   ALA B 356       6.193 -50.178 -53.442  1.00 55.95
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BBBBATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81
BBBBATOM   5274  CB  LEU B 357       6.871 -45.997 -53.290  1.00 58.04
BBBBATOM   5275  CG  LEU B 357       5.595 -45.422 -53.915  1.00 58.29
BBBBATOM   5276  CD1 LEU B 357       5.624 -43.903 -53.820  1.00 58.36
BBBBATOM   5277  CD2 LEU B 357       5.485 -45.859 -55.370  1.00 58.62
BBBBATOM   5278  C   LEU B 357       8.391 -47.895 -52.729  1.00 58.46
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WATR
ATOM   5283  OH2 WAT W   5      20.119 -17.520 -22.473  1.00 21.13
WATR
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WATR
ATOM   5285  OH2 WAT W   7       2.329 -28.724 -15.978  1.00 27.32
WATR
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WATR
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WATR
ATOM   5292  OH2 WAT W  14       4.845 -57.924 -27.444  1.00 24.35
WATR
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WATR
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WATR
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ATOM   5303  OH2 WAT W  25     -29.060  13.621  26.406  1.00 21.08
WATR
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WATR
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ATOM   5314  OH2 WAT W  36       0.540  14.225  10.932  1.00 26.89
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ATOM   5323  OH2 WAT W  45      30.256 -23.202 -11.163  1.00 33.81
WATR
ATOM   5324  OH2 WAT W  46      -6.107 -66.004 -38.690  1.00 30.45
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ATOM   5325  OH2 WAT W  47      17.631 -17.241  -5.864  1.00 28.69
WATR
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ATOM   5352  OH2 WAT W  74      21.404 -42.041 -26.621  1.00 31.41
WATRATOM   5353  OH2 WAT W  75      -1.110 -15.319  -1.089  1.00 31.51
WATRATOM   5354  OH2 WAT W  76       0.688  19.730  22.519  1.00 26.71
WATRATOM   5355  OH2 WAT W  77      12.113 -69.335 -26.593  1.00 27.11
WATRATOM   5356  OH2 WAT W  78      11.725 -25.065 -33.817  1.00 43.79
WATRATOM   5357  OH2 WAT W  79     -25.519   9.450  22.092  1.00 28.18
WATRATOM   5358  OH2 WAT W  80     -14.673   6.584  16.023  1.00 31.37
WATRATOM   5359  OH2 WAT W  81      -2.250  -0.253  -1.741  1.00 29.99
WATRATOM   5360  OH2 WAT W  82      -7.300  12.943   8.415  1.00 32.39
WATRATOM   5361  OH2 WAT W  83       1.712 -13.629 -13.904  1.00 34.08
WATRATOM   5362  OH2 WAT W  84       4.709 -17.478  -6.557  1.00 29.67
WATRATOM   5363  OH2 WAT W  85      10.070 -57.496 -44.450  1.00 48.39
WATRATOM   5364  OH2 WAT W  86       8.040 -30.281 -10.117  1.00 28.59
WATRATOM   5365  OH2 WAT W  87      -1.967 -32.372 -38.643  1.00 31.55
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WATRATOM	5366	OH2	WAT	W	88	-3.178	-64.576	-25.506	1.00	33.66
WATRATOM	5367	OH2	WAT	W	89	15.762	-9.860	-10.400	1.00	34.29
WATRATOM	5368	OH2	WAT	W	90	5.654	-30.990	-27.758	1.00	35.84
WATRATOM	5369	OH2	WAT	W	91	14.959	-46.096	-42.270	1.00	35.21
WATRATOM	5370	OH2	WAT	W	92	10.137	-13.308	-9.753	1.00	32.65
WATRATOM	5371	OH2	WAT	W	93	-4.480	6.624	6.614	1.00	27.37
WATRATOM	5372	OH2	WAT	W	94	-14.574	22.522	18.870	1.00	49.48
WATRATOM	5373	OH2	WAT	W	95	-11.031	-42.768	-39.637	1.00	37.63
WATRATOM	5374	OH2	WAT	W	96	9.906	-35.479	-19.203	1.00	29.59
WATRATOM	5375	OH2	WAT	W	97	-0.990	-0.781	36.951	1.00	37.27
WATRATOM	5376	OH2	WAT	W	98	-11.422	9.059	11.252	1.00	30.43
WATRATOM	5377	OH2	WAT	W	99	8.118	-36.710	-22.371	1.00	34.85
WATRATOM	5378	OH2	WAT	W	100	12.414	-67.326	-22.791	1.00	31.24
WATRATOM	5379	OH2	WAT	W	101	28.541	-24.603	-31.049	1.00	40.14
WATRATOM	5380	OH2	WAT	W	102	16.276	-10.934	-3.673	1.00	33.80
WATRATOM	5381	OH2	WAT	W	103	30.979	-13.264	-22.953	1.00	24.73
WATRATOM	5382	OH2	WAT	W	104	12.759	-31.636	-31.838	1.00	26.40
WATRATOM	5383	OH2	WAT	W	105	23.507	-29.661	-32.187	1.00	29.62
WATRATOM	5384	OH2	WAT	W	106	21.292	-13.141	-24.874	1.00	37.83
WATRATOM	5385	OH2	WAT	W	107	10.171	-32.960	-15.580	1.00	26.59
WATRATOM	5386	OH2	WAT	W	108	-2.207	2.376	2.034	1.00	27.55
WATRATOM	5387	OH2	WAT	W	109	-6.984	22.588	16.082	1.00	39.01
WATRATOM	5388	OH2	WAT	W	110	14.308	-11.038	-15.406	1.00	26.48
WATRATOM	5389	OH2	WAT	W	111	10.612	9.749	24.161	1.00	40.18
WATRATOM	5390	OH2	WAT	W	112	2.406	-15.823	-10.196	1.00	27.61
WATRATOM	5391	OH2	WAT	W	113	6.310	-68.984	-20.661	1.00	40.25
WATRATOM	5392	OH2	WAT	W	114	14.379	-10.930	-8.565	1.00	35.86
WATRATOM	5393	OH2	WAT	W	115	24.183	-35.475	-30.338	1.00	35.17
WATRATOM	5394	OH2	WAT	W	116	21.897	-31.717	-1.243	1.00	47.61
WATRATOM	5395	OH2	WAT	W	117	24.065	-17.545	-13.707	1.00	32.24
WATRATOM	5396	OH2	WAT	W	118	16.772	-51.926	-25.940	1.00	38.66
WATRATOM	5397	OH2	WAT	W	119	-5.862	6.629	4.446	1.00	39.57
WATRATOM	5398	OH2	WAT	W	120	14.133	-57.303	-28.159	1.00	30.19
WATRATOM	5399	OH2	WAT	W	121	-16.538	-6.724	21.638	1.00	40.50
WATRATOM	5400	OH2	WAT	W	122	19.669	-18.487	-33.216	1.00	38.38
WATRATOM	5401	OH2	WAT	W	123	15.481	1.078	-4.048	1.00	32.28
WATRATOM	5402	OH2	WAT	W	124	20.395	-13.033	-2.072	1.00	49.69
WATRATOM	5403	OH2	WAT	W	125	15.526	-1.437	-15.842	1.00	36.06
WATRATOM	5404	OH2	WAT	W	126	7.297	-29.419	-1.509	1.00	34.75
WATRATOM	5405	OH2	WAT	W	127	9.994	-12.069	-21.013	1.00	32.21
WATRATOM	5406	OH2	WAT	W	128	17.433	-42.825	-16.713	1.00	31.02
WATRATOM	5407	OH2	WAT	W	129	-15.855	20.882	21.019	1.00	44.11
WATRATOM	5408	OH2	WAT	W	130	-6.351	-7.687	-14.067	1.00	35.04
WATRATOM	5409	OH2	WAT	W	131	7.954	-17.872	-1.475	1.00	28.45
WATRATOM	5410	OH2	WAT	W	132	13.526	-34.593	-31.844	1.00	31.12
WATRATOM	5411	OH2	WAT	W	133	9.992	-41.228	-23.098	1.00	26.45
WATRATOM	5412	OH2	WAT	W	134	8.434	18.132	16.019	1.00	32.97
WATRATOM	5413	OH2	WAT	W	135	-1.208	-33.658	-36.216	1.00	38.33
WATRATOM	5414	OH2	WAT	W	136	-14.502	9.100	12.433	1.00	43.21
WATRATOM	5415	OH2	WAT	W	137	14.394	-43.675	-17.325	1.00	32.32
WATRATOM	5416	OH2	WAT	W	138	-4.809	-30.333	-46.416	1.00	42.65
WATRATOM	5417	OH2	WAT	W	139	18.861	-35.072	-35.671	1.00	43.56
WATRATOM	5418	OH2	WAT	W	140	-10.162	-60.139	-32.862	1.00	35.41
WATRATOM	5419	OH2	WAT	W	141	6.740	-32.411	-35.303	1.00	38.57
WATRATOM	5420	OH2	WAT	W	142	-12.257	-60.854	-39.307	1.00	32.90
WATRATOM	5421	OH2	WAT	W	143	18.910	-40.984	-13.084	1.00	43.43
WATRATOM	5422	OH2	WAT	W	144	18.857	-49.375	-28.645	1.00	31.34
WATRATOM	5423	OH2	WAT	W	145	0.235	-17.424	-16.608	1.00	38.85
WATRATOM	5424	OH2	WAT	W	146	14.236	-11.252	-24.086	1.00	27.79
WATRATOM	5425	OH2	WAT	W	147	31.513	-22.336	-22.128	1.00	43.18
WATRATOM	5426	OH2	WAT	W	148	-5.314	-70.396	-26.090	1.00	43.91
WATRATOM	5427	OH2	WAT	W	149	-7.717	-64.969	-36.808	1.00	26.30
WATRATOM	5428	OH2	WAT	W	150	22.584	-12.594	-4.179	1.00	46.91
WATRATOM	5429	OH2	WAT	W	151	-12.388	9.493	36.619	1.00	32.82
WATRATOM	5430	OH2	WAT	W	152	-14.517	16.479	37.760	1.00	39.52
WATRATOM	5431	OH2	WAT	W	153	-10.095	-34.647	-29.068	1.00	41.08

WATRATOM	5432	OH2	WAT	W	154	-5.233	-4.134	31.160	1.00 35.31
WATRATOM	5433	OH2	WAT	W	155	-6.322	11.278	-1.883	1.00 35.75
WATRATOM	5434	OH2	WAT	W	156	10.262	-9.572	-16.736	1.00 42.40
WATRATOM	5435	OH2	WAT	W	157	22.929	-10.414	-23.566	1.00 36.66
WATRATOM	5436	OH2	WAT	W	158	-15.987	3.994	16.559	1.00 37.22
WATRATOM	5437	OH2	WAT	W	159	13.385	-44.923	-46.826	1.00 41.55
WATRATOM	5438	OH2	WAT	W	160	26.508	-13.616	-18.049	1.00 25.93
WATRATOM	5439	OH2	WAT	W	161	4.671	-66.907	-17.861	1.00 31.54
WATRATOM	5440	OH2	WAT	W	162	-12.589	12.262	11.825	1.00 32.71
WATRATOM	5441	OH2	WAT	W	163	13.899	-62.269	-25.144	1.00 30.71
WATRATOM	5442	OH2	WAT	W	164	-31.053	15.663	19.272	1.00 30.19
WATRATOM	5443	OH2	WAT	W	165	9.797	-47.899	-25.140	1.00 26.79
WATRATOM	5444	OH2	WAT	W	166	0.877	-51.774	-25.619	1.00 30.02
WATRATOM	5445	OH2	WAT	W	167	-17.088	16.246	37.180	1.00 25.63
WATRATOM	5446	OH2	WAT	W	168	0.855	-52.086	-22.078	1.00 40.99
WATRATOM	5447	OH2	WAT	W	169	-14.873	18.295	21.203	1.00 40.28
WATRATOM	5448	OH2	WAT	W	170	11.913	-62.134	-35.641	1.00 41.33
WATRATOM	5449	OH2	WAT	W	171	25.783	-23.984	-33.162	1.00 44.03
WATRATOM	5450	OH2	WAT	W	172	7.169	-50.047	-23.737	1.00 47.85
WATRATOM	5451	OH2	WAT	W	173	20.074	-42.845	-14.939	1.00 32.87
WATRATOM	5452	OH2	WAT	W	174	8.765	5.909	9.193	1.00 34.30
WATRATOM	5453	OH2	WAT	W	175	-4.953	-64.494	-45.351	1.00 47.11
WATRATOM	5454	OH2	WAT	W	176	11.889	-61.263	-22.531	1.00 36.63
WATRATOM	5455	OH2	WAT	W	177	2.149	-49.169	-24.836	1.00 39.21
WATRATOM	5456	OH2	WAT	W	178	-14.051	6.399	13.353	1.00 39.89
WATRATOM	5457	OH2	WAT	W	179	8.488	-46.760	-23.118	1.00 45.24
WATRATOM	5458	OH2	WAT	W	180	-1.152	-23.348	-11.975	1.00 30.36
WATRATOM	5459	OH2	WAT	W	181	-7.002	3.531	7.051	1.00 44.50
WATRATOM	5460	OH2	WAT	W	182	-12.320	-54.772	-29.990	1.00 38.61
WATRATOM	5461	OH2	WAT	W	183	6.790	-54.559	-47.733	1.00 44.05
WATRATOM	5462	OH2	WAT	W	184	26.305	-38.240	-19.177	1.00 39.53
WATRATOM	5463	OH2	WAT	W	185	20.402	-58.179	-34.391	1.00 46.11
WATRATOM	5464	OH2	WAT	W	186	8.061	-31.341	-19.653	1.00 41.37
WATRATOM	5465	OH2	WAT	W	187	-7.549	-15.619	-5.482	1.00 40.60
WATRATOM	5466	OH2	WAT	W	188	-31.099	11.941	25.471	1.00 38.80
WATRATOM	5467	OH2	WAT	W	189	28.566	-25.441	-15.103	1.00 34.75
WATRATOM	5468	OH2	WAT	W	190	-5.613	-40.109	-50.158	1.00 49.21
WATRATOM	5469	OH2	WAT	W	191	17.024	-13.428	1.709	1.00 39.93
WATRATOM	5470	OH2	WAT	W	192	-22.114	10.176	37.673	1.00 32.53
WATRATOM	5471	OH2	WAT	W	193	10.204	-29.330	-20.066	1.00 27.24
WATRATOM	5472	OH2	WAT	W	194	27.893	-25.793	-21.862	1.00 38.97
WATRATOM	5473	OH2	WAT	W	195	-5.582	17.681	32.898	1.00 43.64
WATRATOM	5474	OH2	WAT	W	196	23.004	-45.224	-27.870	1.00 43.04
WATRATOM	5475	OH2	WAT	W	197	5.189	-58.857	-25.016	1.00 28.15
WATRATOM	5476	OH2	WAT	W	198	-7.740	-56.165	-24.052	1.00 35.98
WATRATOM	5477	OH2	WAT	W	199	-8.156	24.723	26.733	1.00 45.54
WATRATOM	5478	OH2	WAT	W	200	23.286	-32.333	-33.400	1.00 38.12
WATRATOM	5479	OH2	WAT	W	201	30.646	-14.180	-20.528	1.00 31.01
WATRATOM	5480	OH2	WAT	W	202	-8.238	-4.609	29.299	1.00 39.76
WATRATOM	5481	OH2	WAT	W	203	19.370	0.814	-7.532	1.00 35.83
WATRATOM	5482	OH2	WAT	W	204	0.885	-27.619	-1.442	1.00 47.04
WATRATOM	5483	OH2	WAT	W	205	16.084	-56.649	-26.382	1.00 45.97
WATRATOM	5484	OH2	WAT	W	206	-0.698	-19.360	-9.869	1.00 37.53
WATRATOM	5485	OH2	WAT	W	207	0.682	-14.985	-15.794	1.00 33.35
WATRATOM	5486	OH2	WAT	W	208	1.646	17.427	31.991	1.00 40.39
WATRATOM	5487	OH2	WAT	W	209	-21.611	1.533	20.359	1.00 31.04
WATRATOM	5488	OH2	WAT	W	210	-5.143	-55.137	-45.825	1.00 30.17
WATRATOM	5489	OH2	WAT	W	211	-9.645	13.045	37.660	1.00 42.93
WATRATOM	5490	OH2	WAT	W	212	22.096	-11.242	-30.224	1.00 48.12
WATRATOM	5491	OH2	WAT	W	213	-5.759	2.610	-15.984	1.00 41.67
WATRATOM	5492	OH2	WAT	W	214	-4.323	7.731	-7.331	1.00 37.92
WATRATOM	5493	OH2	WAT	W	215	-5.450	7.197	10.632	1.00 33.99
WATRATOM	5494	OH2	WAT	W	216	2.330	-32.635	-34.500	1.00 38.85
WATRATOM	5495	OH2	WAT	W	217	-26.827	16.219	13.451	1.00 38.12
WATRATOM	5496	OH2	WAT	W	218	10.887	-51.427	-23.191	1.00 39.81
WATRATOM	5497	OH2	WAT	W	219	-9.020	19.746	-3.698	1.00 46.58

WATRATOM	5498	OH2	WAT	W	220	9.054	6.622	-0.709	1.00	34.14
WATRATOM	5499	OH2	WAT	W	221	4.173	-7.985	-23.786	1.00	32.75
WATRATOM	5500	OH2	WAT	W	222	0.983	16.806	3.910	1.00	40.83
WATRATOM	5501	OH2	WAT	W	223	2.222	-16.848	-6.783	1.00	33.50
WATRATOM	5502	OH2	WAT	W	224	13.627	1.072	-15.114	1.00	37.51
WATRATOM	5503	OH2	WAT	W	225	12.533	-14.212	-9.007	1.00	38.40
WATRATOM	5504	OH2	WAT	W	226	1.404	-7.852	5.396	1.00	38.55
WATRATOM	5505	OH2	WAT	W	227	31.159	-24.354	-31.143	1.00	37.67
WATRATOM	5506	OH2	WAT	W	228	-13.047	-60.728	-42.282	1.00	42.18
WATRATOM	5507	OH2	WAT	W	229	8.956	-37.681	-16.765	1.00	41.45
WATRATOM	5508	OH2	WAT	W	230	28.749	-13.637	-16.860	1.00	42.34
WATRATOM	5509	OH2	WAT	W	231	-4.461	19.451	8.684	1.00	36.17
WATRATOM	5510	OH2	WAT	W	232	-9.785	-66.504	-35.701	1.00	44.07
WATRATOM	5511	OH2	WAT	W	233	10.673	-41.619	-20.678	1.00	36.58
WATRATOM	5512	OH2	WAT	W	234	-15.694	1.684	32.613	1.00	44.04
WATRATOM	5513	OH2	WAT	W	235	3.345	1.229	9.738	1.00	35.70
WATRATOM	5514	OH2	WAT	W	236	-6.256	-68.913	-30.401	1.00	36.72
WATRATOM	5515	OH2	WAT	W	237	28.344	-21.326	-30.399	1.00	36.45
WATRATOM	5516	OH2	WAT	W	238	2.876	-34.368	-17.344	1.00	42.48
WATRATOM	5517	OH2	WAT	W	239	15.355	-11.202	2.371	1.00	38.84
WATRATOM	5518	OH2	WAT	W	240	27.066	-22.336	-6.437	1.00	37.37
WATRATOM	5519	OH2	WAT	W	241	2.222	18.464	26.994	1.00	35.75
WATRATOM	5520	OH2	WAT	W	242	15.052	-9.829	-31.019	1.00	44.31
WATRATOM	5521	OH2	WAT	W	243	10.351	-67.649	-21.184	1.00	35.79
WATRATOM	5522	OH2	WAT	W	244	-13.173	14.269	38.605	1.00	41.50
WATRATOM	5523	OH2	WAT	W	245	-7.569	9.658	0.793	1.00	37.62
WATRATOM	5524	OH2	WAT	W	246	-2.167	-47.395	-19.605	1.00	45.90
WATRATOM	5525	OH2	WAT	W	247	7.166	2.400	15.830	1.00	42.90
WATRATOM	5526	OH2	WAT	W	248	-11.231	-10.901	-10.057	1.00	45.28
WATRATOM	5527	OH2	WAT	W	249	5.684	-16.094	-26.796	1.00	44.76
WATRATOM	5528	OH2	WAT	W	250	-4.745	3.667	-18.932	1.00	46.20
WATRATOM	5529	OH2	WAT	W	251	-0.505	-22.136	-9.079	1.00	42.89
WATRATOM	5530	OH2	WAT	W	252	16.668	-37.987	-7.767	1.00	35.76
WATRATOM	5531	OH2	WAT	W	253	2.454	-18.256	-26.130	1.00	43.33
WATRATOM	5532	OH2	WAT	W	254	-8.367	-39.960	-21.638	1.00	43.07
WATRATOM	5533	OH2	WAT	W	255	15.642	7.805	9.633	1.00	47.78
WATRATOM	5534	OH2	WAT	W	256	13.660	-24.331	1.932	1.00	42.50
WATRATOM	5535	OH2	WAT	W	257	11.567	-6.104	-23.359	1.00	37.10
WATRATOM	5536	OH2	WAT	W	258	18.941	-16.698	0.528	1.00	40.97
WATRATOM	5537	OH2	WAT	W	259	-11.441	-63.514	-39.126	1.00	43.17
WATRATOM	5538	OH2	WAT	W	260	28.664	-39.605	-22.853	1.00	42.65
WATRATOM	5539	OH2	WAT	W	261	6.795	-6.961	31.114	1.00	38.28
WATRATOM	5540	OH2	WAT	W	262	7.077	-14.349	-24.858	1.00	41.00
WATRATOM	5541	OH2	WAT	W	263	-2.259	-48.991	-29.099	1.00	34.96
WATRATOM	5542	OH2	WAT	W	264	21.812	-44.128	-35.641	1.00	44.51
WATRATOM	5543	OH2	WAT	W	265	-27.570	4.389	13.296	1.00	48.63
WATRATOM	5544	OH2	WAT	W	266	13.573	-27.185	0.220	1.00	43.56
WATRATOM	5545	OH2	WAT	W	267	16.549	8.451	-13.582	1.00	44.84
WATRATOM	5546	OH2	WAT	W	268	-9.142	9.107	36.872	1.00	37.66
WATRATOM	5547	OH2	WAT	W	269	5.648	-11.797	-24.893	1.00	45.79
WATRATOM	5548	OH2	WAT	W	270	3.619	-14.850	-23.652	1.00	34.09
WATRATOM	5549	OH2	WAT	W	271	-8.129	-11.098	-16.064	1.00	39.37
WATRATOM	5550	OH2	WAT	W	272	-17.342	8.563	9.979	1.00	46.38
WATRATOM	5551	OH2	WAT	W	273	8.798	-36.348	-46.119	1.00	37.71
WATRATOM	5552	OH2	WAT	W	274	9.190	-10.509	-35.865	1.00	45.80
WATRATOM	5553	OH2	WAT	W	275	13.545	-13.441	3.898	1.00	42.83
WATRATOM	5554	OH2	WAT	W	276	-7.844	0.944	-2.560	1.00	46.27
WATRATOM	5555	OH2	WAT	W	277	0.478	-47.721	-55.170	1.00	46.25
WATRATOM	5556	OH2	WAT	W	278	24.658	-18.359	-11.005	1.00	36.33
WATRATOM	5557	OH2	WAT	W	279	-4.675	21.561	12.155	1.00	37.17
WATRATOM	5558	OH2	WAT	W	280	0.382	20.486	4.930	1.00	41.40
WATRATOM	5559	OH2	WAT	W	281	5.919	18.010	25.033	1.00	41.72
WATRATOM	5560	OH2	WAT	W	282	-2.987	-63.751	-22.983	1.00	43.76
WATRATOM	5561	OH2	WAT	W	283	8.990	-33.134	-17.898	1.00	40.17
WATRATOM	5562	OH2	WAT	W	284	0.155	-61.872	-48.384	1.00	49.87
WATRATOM	5563	OH2	WAT	W	285	-10.443	-56.965	-24.681	1.00	48.02

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WATRATOM    5564   OH2 WAT W 286      18.915 -33.048  -3.930  1.00 37.81
WATRATOM    5565   OH2 WAT W 287     -16.181  11.706  12.277  1.00 41.77
WATRATOM    5566   OH2 WAT W 288       7.197   7.180  10.953  1.00 46.19
WATRATOM    5567   OH2 WAT W 289      31.934 -26.155 -26.053  1.00 38.77
WATRATOM    5568   OH2 WAT W 290     -15.232  -0.248  11.315  1.00 40.14
WATRATOM    5569   OH2 WAT W 291       9.450 -27.963  -1.396  1.00 41.29
WATRATOM    5570   OH2 WAT W 292      -1.800  13.139  -9.983  1.00 41.60
WATRATOM    5571   OH2 WAT W 293      -7.766   5.988   9.798  1.00 40.11
WATRATOM    5572   OH2 WAT W 294       7.973   4.338  14.321  1.00 39.97
WATRATOM    5573   OH2 WAT W 295      23.449 -40.563 -27.347  1.00 40.59
WATRATOM    5574   OH2 WAT W 296      -3.537 -28.260 -15.925  1.00 42.10
WATRATOM    5575   OH2 WAT W 297      28.052 -32.620 -12.168  1.00 48.03
WATRATOM    5576   OH2 WAT W 298      20.655 -43.315 -28.829  1.00 40.17
WATR
ATOM    5577  S    SO4 S   1        1.273 -70.953 -23.009  1.00 22.99
SO4
ATOM    5578  O1   SO4 S   1        1.720 -71.882 -24.053  1.00 21.18
SO4
ATOM    5579  O2   SO4 S   1        0.908 -69.659 -23.626  1.00 22.47
SO4
ATOM    5580  O3   SO4 S   1        2.337 -70.752 -22.018  1.00 23.88
SO4
ATOM    5581  O4   SO4 S   1        0.088 -71.522 -22.328  1.00 22.50
SO4
TEREND
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TABLE 2 ATOMIC COORDINATES OF E.COLI MURG C-ALPHA BACKBONE ATOMS

ATOM	2649	CA	LYS	B	7	-6.512	-45.403	-47.519	1.00	45.28	BBBB
ATOM	2651	CA	ARG	B	8	-6.682	-47.303	-44.240	1.00	38.63	BBBB
ATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00	30.88	BBBB
ATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00	26.66	BBBB
ATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00	23.16	BBBB
ATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	BBBB
ATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00	29.43	BBBB
ATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00	33.82	BBBB
ATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00	36.08	BBBB
ATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00	38.51	BBBB
ATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00	36.57	BBBB
ATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00	33.48	BBBB
ATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00	28.22	BBBB
ATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00	27.77	BBBB
ATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00	29.00	BBBB
ATOM	2750	CA	PRO	B	22	2.986	-39.252	-31.086	1.00	26.12	BBBB
ATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00	25.07	BBBB
ATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00	25.32	BBBB
ATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00	25.94	BBBB
ATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00	25.70	BBBB
ATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00	26.15	BBBB
ATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00	29.32	BBBB
ATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00	32.38	BBBB
ATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00	32.00	BBBB
ATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00	34.91	BBBB
ATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00	37.55	BBBB
ATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00	38.24	BBBB
ATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00	35.75	BBBB
ATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00	34.58	BBBB
ATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00	35.40	BBBB
ATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00	34.16	BBBB
ATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00	31.56	BBBB
ATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00	27.41	BBBB
ATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71	BBBB
ATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00	23.47	BBBB
ATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00	29.84	BBBB
ATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00	38.81	BBBB
ATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00	44.47	BBBB
ATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00	40.44	BBBB
ATOM	2937	CA	MET	B	46	-4.881	-45.581	-21.249	1.00	36.33	BBBB
ATOM	2945	CA	GLU	B	47	-5.458	-45.655	-25.029	1.00	31.79	BBBB
ATOM	2954	CA	ALA	B	48	-8.821	-47.344	-24.414	1.00	32.58	BBBB
ATOM	2959	CA	ASP	B	49	-10.143	-44.065	-23.009	1.00	35.60	BBBB
ATOM	2967	CA	LEU	B	50	-8.026	-41.484	-24.840	1.00	33.49	BBBB
ATOM	2975	CA	VAL	B	51	-8.299	-42.641	-28.449	1.00	32.68	BBBB
ATOM	2983	CA	PRO	B	52	-12.111	-42.601	-28.453	1.00	34.43	BBBB
ATOM	2989	CA	LYS	B	53	-11.998	-39.054	-27.064	1.00	36.73	BBBB
ATOM	2998	CA	HIS	B	54	-10.116	-38.212	-30.259	1.00	34.62	BBBB
ATOM	3008	CA	GLY	B	55	-12.938	-39.481	-32.447	1.00	35.34	BBBB
ATOM	3012	CA	ILE	B	56	-10.909	-42.517	-33.514	1.00	33.81	BBBB
ATOM	3020	CA	GLU	B	57	-12.228	-46.083	-33.467	1.00	34.16	BBBB
ATOM	3029	CA	ILE	B	58	-10.217	-48.658	-31.553	1.00	31.38	BBBB
ATOM	3037	CA	ASP	B	59	-10.039	-52.442	-31.720	1.00	31.09	BBBB
ATOM	3045	CA	PHE	B	60	-8.809	-54.410	-28.713	1.00	30.32	BBBB
ATOM	3056	CA	ILE	B	61	-6.832	-57.616	-28.269	1.00	28.55	BBBB
ATOM	3064	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00	30.76	BBBB
ATOM	3075	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	BBBB
ATOM	3083	CA	SER	B	64	-2.356	-60.520	-20.505	1.00	37.51	BBBB
ATOM	3089	CA	GLY	B	65	0.679	-62.355	-19.199	1.00	37.13	BBBB
ATOM	3093	CA	LEU	B	66	2.591	-61.413	-22.355	1.00	33.17	BBBB
ATOM	3101	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	BBBB

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ATOM   3112  CA  GLY B  68       7.380 -57.427 -20.685  1.00 26.79 BBBB
ATOM   3116  CA  LYS B  69       8.238 -60.463 -22.796  1.00 23.93 BBBB
ATOM   3125  CA  GLY B  70      10.755 -60.229 -25.636  1.00 22.26 BBBB
ATOM   3129  CA  ILE B  71      10.357 -62.386 -28.762  1.00 23.55 BBBB
ATOM   3137  CA  LYS B  72      12.038 -65.491 -27.343  1.00 24.92 BBBB
ATOM   3146  CA  ALA B  73       9.839 -65.306 -24.233  1.00 21.18 BBBB
ATOM   3151  CA  LEU B  74       6.745 -64.762 -26.387  1.00 19.36 BBBB
ATOM   3159  CA  ILE B  75       7.434 -67.768 -28.601  1.00 21.18 BBBB
ATOM   3167  CA  ALA B  76       7.996 -69.726 -25.374  1.00 21.72 BBBB
ATOM   3172  CA  ALA B  77       4.289 -69.121 -24.655  1.00 21.07 BBBB
ATOM   3178  CA  PRO B  78       2.772 -70.846 -27.771  1.00 20.95 BBBB
ATOM   3184  CA  LEU B  79      -0.896 -70.728 -26.783  1.00 21.32 BBBB
ATOM   3192  CA  ARG B  80      -0.980 -67.115 -25.637  1.00 21.30 BBBB
ATOM   3203  CA  ILE B  81       1.113 -65.621 -28.421  1.00 19.47 BBBB
ATOM   3211  CA  PHE B  82      -0.875 -67.582 -31.038  1.00 19.15 BBBB
ATOM   3222  CA  ASN B  83      -4.150 -66.332 -29.577  1.00 20.90 BBBB
ATOM   3230  CA  ALA B  84      -3.177 -62.647 -29.484  1.00 19.30 BBBB
ATOM   3235  CA  TRP B  85      -1.820 -63.111 -33.032  1.00 20.56 BBBB
ATOM   3249  CA  ARG B  86      -5.140 -64.660 -34.166  1.00 23.28 BBBB
ATOM   3260  CA  GLN B  87      -7.101 -61.802 -32.567  1.00 24.07 BBBB
ATOM   3269  CA  ALA B  88      -4.996 -59.183 -34.355  1.00 23.78 BBBB
ATOM   3274  CA  ARG B  89      -5.285 -61.111 -37.636  1.00 24.94 BBBB
ATOM   3285  CA  ALA B  90      -9.088 -61.151 -37.383  1.00 26.16 BBBB
ATOM   3290  CA  ILE B  91      -9.108 -57.400 -36.733  1.00 26.97 BBBB
ATOM   3298  CA  MET B  92      -6.872 -56.693 -39.717  1.00 29.03 BBBB
ATOM   3306  CA  LYS B  93      -8.735 -59.038 -42.050  1.00 33.20 BBBB
ATOM   3315  CA  ALA B  94     -11.943 -57.157 -41.183  1.00 33.62 BBBB
ATOM   3320  CA  TYR B  95     -10.504 -53.620 -41.224  1.00 33.83 BBBB
ATOM   3332  CA  LYS B  96      -8.104 -54.327 -44.122  1.00 33.85 BBBB
ATOM   3342  CA  PRO B  97      -5.490 -51.623 -43.419  1.00 31.82 BBBB
ATOM   3348  CA  ASP B  98      -3.049 -50.685 -46.188  1.00 29.78 BBBB
ATOM   3356  CA  VAL B  99      -0.296 -50.214 -43.660  1.00 26.75 BBBB
ATOM   3363  CA  VAL B 100       0.227 -50.613 -39.936  1.00 23.59 BBBB
ATOM   3370  CA  LEU B 101       2.214 -48.199 -37.797  1.00 21.59 BBBB
ATOM   3378  CA  GLY B 102       3.796 -49.357 -34.549  1.00 19.23 BBBB
ATOM   3382  CA  MET B 103       4.892 -46.597 -32.191  1.00 18.93 BBBB
ATOM   3390  CA  GLY B 104       6.275 -49.080 -29.686  1.00 21.89 BBBB
ATOM   3394  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54 BBBB
ATOM   3398  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37 BBBB
ATOM   3410  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06 BBBB
ATOM   3417  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67 BBBB
ATOM   3423  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03 BBBB
ATOM   3428  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99 BBBB
ATOM   3434  CA  GLY B 111      -0.160 -56.702 -34.025  1.00 19.60 BBBB
ATOM   3438  CA  GLY B 112       3.014 -56.417 -36.074  1.00 19.97 BBBB
ATOM   3442  CA  LEU B 113       3.265 -60.184 -36.429  1.00 19.49 BBBB
ATOM   3450  CA  ALA B 114      -0.334 -60.292 -37.661  1.00 18.70 BBBB
ATOM   3455  CA  ALA B 115       0.167 -57.516 -40.229  1.00 21.84 BBBB
ATOM   3460  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22 BBBB
ATOM   3474  CA  SER B 117       1.735 -62.573 -41.873  1.00 22.61 BBBB
ATOM   3480  CA  LEU B 118      -1.069 -60.957 -43.882  1.00 25.70 BBBB
ATOM   3488  CA  GLY B 119       1.354 -59.174 -46.192  1.00 27.80 BBBB
ATOM   3492  CA  ILE B 120       0.568 -55.744 -44.731  1.00 24.85 BBBB
ATOM   3501  CA  PRO B 121       3.625 -53.477 -44.591  1.00 22.63 BBBB
ATOM   3507  CA  VAL B 122       4.743 -52.594 -41.083  1.00 22.03 BBBB
ATOM   3514  CA  VAL B 123       6.200 -49.184 -40.310  1.00 20.82 BBBB
ATOM   3521  CA  LEU B 124       7.749 -48.485 -36.915  1.00 22.10 BBBB
ATOM   3529  CA  HIS B 125       8.814 -45.413 -34.981  1.00 21.42 BBBB
ATOM   3539  CA  GLU B 126      10.947 -45.452 -31.817  1.00 22.15 BBBB
ATOM   3548  CA  GLN B 127      10.682 -42.270 -29.735  1.00 22.81 BBBB
ATOM   3557  CA  ASN B 128      13.406 -43.097 -27.216  1.00 22.96 BBBB
ATOM   3565  CA  GLY B 129      17.203 -43.019 -27.294  1.00 25.36 BBBB
ATOM   3569  CA  ILE B 130      17.160 -46.716 -26.488  1.00 28.00 BBBB
ATOM   3577  CA  ALA B 131      14.978 -49.139 -28.461  1.00 25.89 BBBB
ATOM   3582  CA  GLY B 132      12.007 -50.532 -26.568  1.00 24.05 BBBB
ATOM   3586  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54 BBBB
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ATOM   3594  CA  THR B 134     9.202 -54.860 -28.639  1.00 21.22 BBBB
ATOM   3601  CA  ASN B 135    10.407 -52.419 -31.324  1.00 20.50 BBBB
ATOM   3609  CA  LYS B 136    13.886 -53.949 -31.144  1.00 22.79 BBBB
ATOM   3618  CA  TRP B 137    12.753 -57.345 -32.424  1.00 22.06 BBBB
ATOM   3632  CA  LEU B 138     9.744 -56.188 -34.431  1.00 23.15 BBBB
ATOM   3640  CA  ALA B 139    12.128 -54.092 -36.542  1.00 25.29 BBBB
ATOM   3645  CA  LYS B 140    13.279 -57.337 -38.182  1.00 28.05 BBBB
ATOM   3654  CA  ILE B 141     9.963 -57.818 -40.016  1.00 26.09 BBBB
ATOM   3662  CA  ALA B 142     9.331 -54.107 -40.498  1.00 25.03 BBBB
ATOM   3667  CA  THR B 143     9.262 -52.595 -43.984  1.00 26.10 BBBB
ATOM   3674  CA  LYS B 144    10.436 -49.238 -42.618  1.00 24.73 BBBB
ATOM   3683  CA  VAL B 145    11.947 -48.311 -39.252  1.00 23.62 BBBB
ATOM   3690  CA  MET B 146    12.338 -44.736 -37.993  1.00 23.15 BBBB
ATOM   3698  CA  GLN B 147    13.762 -43.418 -34.712  1.00 25.05 BBBB
ATOM   3707  CA  ALA B 148    13.559 -40.032 -33.009  1.00 26.88 BBBB
ATOM   3712  CA  PHE B 149    17.239 -39.820 -32.098  1.00 29.39 BBBB
ATOM   3724  CA  PRO B 150    20.310 -41.541 -33.535  1.00 31.87 BBBB
ATOM   3730  CA  GLY B 151    21.629 -44.537 -31.595  1.00 32.62 BBBB
ATOM   3734  CA  ALA B 152    18.447 -46.476 -30.753  1.00 32.71 BBBB
ATOM   3739  CA  PHE B 153    18.925 -48.506 -33.937  1.00 34.83 BBBB
ATOM   3751  CA  PRO B 154    22.158 -48.751 -35.993  1.00 38.97 BBBB
ATOM   3757  CA  ASN B 155    20.765 -47.568 -39.346  1.00 41.08 BBBB
ATOM   3765  CA  ALA B 156    17.170 -46.407 -38.843  1.00 37.55 BBBB
ATOM   3770  CA  GLU B 157    16.367 -43.044 -40.460  1.00 34.40 BBBB
ATOM   3779  CA  VAL B 158    16.337 -40.344 -37.764  1.00 31.16 BBBB
ATOM   3786  CA  VAL B 159    13.155 -38.265 -37.889  1.00 28.10 BBBB
ATOM   3793  CA  GLY B 160    12.724 -36.921 -34.355  1.00 26.93 BBBB
ATOM   3797  CA  ASN B 161     9.456 -36.807 -32.375  1.00 25.27 BBBB
ATOM   3806  CA  PRO B 162     6.315 -34.747 -33.004  1.00 26.14 BBBB
ATOM   3812  CA  VAL B 163     6.456 -31.379 -31.216  1.00 27.75 BBBB
ATOM   3819  CA  ARG B 164     3.667 -28.953 -30.246  1.00 32.36 BBBB
ATOM   3830  CA  THR B 165     3.038 -26.307 -32.924  1.00 31.74 BBBB
ATOM   3837  CA  ASP B 166     3.252 -23.404 -30.466  1.00 30.64 BBBB
ATOM   3845  CA  VAL B 167     6.746 -24.503 -29.440  1.00 25.91 BBBB
ATOM   3852  CA  LEU B 168     7.780 -25.002 -33.075  1.00 28.46 BBBB
ATOM   3860  CA  ALA B 169     6.580 -21.455 -33.756  1.00 31.43 BBBB
ATOM   3865  CA  LEU B 170     9.002 -19.905 -31.268  1.00 29.60 BBBB
ATOM   3874  CA  PRO B 171    11.611 -17.457 -32.642  1.00 30.11 BBBB
ATOM   3880  CA  LEU B 172    15.157 -18.780 -33.062  1.00 28.33 BBBB
ATOM   3889  CA  PRO B 173    17.450 -18.550 -29.977  1.00 25.25 BBBB
ATOM   3895  CA  GLN B 174    19.526 -15.527 -31.049  1.00 25.46 BBBB
ATOM   3904  CA  GLN B 175    16.365 -13.525 -31.718  1.00 28.47 BBBB
ATOM   3913  CA  ARG B 176    14.611 -14.635 -28.525  1.00 29.01 BBBB
ATOM   3924  CA  LEU B 177    17.673 -13.970 -26.331  1.00 29.90 BBBB
ATOM   3932  CA  ALA B 178    18.766 -10.776 -28.131  1.00 30.78 BBBB
ATOM   3937  CA  GLY B 179    19.846  -7.993 -25.784  1.00 30.10 BBBB
ATOM   3941  CA  ARG B 180    18.676  -9.965 -22.787  1.00 28.97 BBBB
ATOM   3952  CA  GLU B 181    20.545  -9.027 -19.621  1.00 31.79 BBBB
ATOM   3961  CA  GLY B 182    19.871  -9.586 -15.943  1.00 27.75 BBBB
ATOM   3966  CA  PRO B 183    19.450 -12.832 -13.913  1.00 22.93 BBBB
ATOM   3972  CA  VAL B 184    19.524 -16.146 -15.729  1.00 18.01 BBBB
ATOM   3979  CA  ARG B 185    15.873 -17.216 -16.011  1.00 17.62 BBBB
ATOM   3990  CA  VAL B 186    15.508 -20.771 -14.741  1.00 16.47 BBBB
ATOM   3997  CA  LEU B 187    12.361 -22.710 -15.604  1.00 16.75 BBBB
ATOM   4005  CA  VAL B 188    11.774 -25.775 -13.381  1.00 18.41 BBBB
ATOM   4012  CA  VAL B 189     9.298 -28.234 -14.948  1.00 22.11 BBBB
ATOM   4019  CA  GLY B 190     7.914 -31.188 -12.994  1.00 27.28 BBBB
ATOM   4023  CA  GLY B 191     4.935 -32.163 -15.115  1.00 31.94 BBBB
ATOM   4027  CA  SER B 192     1.313 -32.665 -14.064  1.00 35.91 BBBB
ATOM   4033  CA  GLN B 193     2.292 -34.763 -11.033  1.00 38.53 BBBB
ATOM   4042  CA  GLY B 194     5.398 -32.711 -10.350  1.00 35.02 BBBB
ATOM   4046  CA  ALA B 195     8.977 -33.819  -9.709  1.00 33.12 BBBB
ATOM   4051  CA  ARG B 196     9.538 -34.512  -6.010  1.00 32.63 BBBB
ATOM   4062  CA  ILE B 197    13.329 -34.168  -6.164  1.00 28.10 BBBB
ATOM   4070  CA  LEU B 198    13.069 -30.833  -8.003  1.00 26.58 BBBB
ATOM   4078  CA  ASN B 199    10.497 -29.447  -5.563  1.00 27.07 BBBB
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ATOM	4086	CA	GLN	B	200	12.955	-30.326	-2.794	1.00	30.10	BBBB
ATOM	4095	CA	THR	B	201	16.215	-29.345	-4.474	1.00	27.34	BBBB
ATOM	4102	CA	MET	B	202	15.567	-26.048	-6.268	1.00	23.68	BBBB
ATOM	4111	CA	PRO	B	203	14.608	-23.963	-3.220	1.00	23.84	BBBB
ATOM	4117	CA	GLN	B	204	18.033	-24.708	-1.684	1.00	26.34	BBBB
ATOM	4126	CA	VAL	B	205	19.672	-24.033	-5.043	1.00	24.44	BBBB
ATOM	4133	CA	ALA	B	206	17.980	-20.610	-5.013	1.00	22.84	BBBB
ATOM	4138	CA	ALA	B	207	19.442	-19.857	-1.576	1.00	26.65	BBBB
ATOM	4143	CA	LYS	B	208	22.915	-20.595	-2.919	1.00	28.31	BBBB
ATOM	4152	CA	LEU	B	209	22.577	-18.640	-6.171	1.00	25.68	BBBB
ATOM	4160	CA	GLY	B	210	20.675	-15.628	-4.804	1.00	26.56	BBBB
ATOM	4164	CA	ASP	B	211	20.370	-12.647	-7.190	1.00	28.28	BBBB
ATOM	4172	CA	SER	B	212	22.098	-14.474	-10.067	1.00	25.73	BBBB
ATOM	4178	CA	VAL	B	213	18.925	-16.308	-11.116	1.00	20.76	BBBB
ATOM	4185	CA	THR	B	214	15.204	-15.726	-11.337	1.00	19.60	BBBB
ATOM	4192	CA	ILE	B	215	13.076	-18.850	-11.169	1.00	18.75	BBBB
ATOM	4200	CA	TRP	B	216	9.661	-19.973	-12.378	1.00	19.34	BBBB
ATOM	4214	CA	HIS	B	217	9.015	-23.303	-10.680	1.00	21.06	BBBB
ATOM	4224	CA	GLN	B	218	6.149	-25.594	-11.735	1.00	24.30	BBBB
ATOM	4233	CA	SER	B	219	5.463	-27.800	-8.684	1.00	26.73	BBBB
ATOM	4239	CA	GLY	B	220	2.855	-30.242	-9.961	1.00	30.53	BBBB
ATOM	4243	CA	LYS	B	221	-0.657	-30.914	-8.628	1.00	35.12	BBBB
ATOM	4252	CA	GLY	B	222	-1.195	-29.899	-5.011	1.00	35.34	BBBB
ATOM	4256	CA	SER	B	223	2.451	-28.934	-4.418	1.00	33.98	BBBB
ATOM	4262	CA	GLN	B	224	2.187	-25.208	-5.186	1.00	33.71	BBBB
ATOM	4271	CA	GLN	B	225	1.823	-24.239	-1.519	1.00	32.32	BBBB
ATOM	4280	CA	SER	B	226	4.701	-26.309	-0.122	1.00	28.30	BBBB
ATOM	4286	CA	VAL	B	227	7.214	-25.247	-2.791	1.00	24.28	BBBB
ATOM	4293	CA	GLU	B	228	6.178	-21.592	-2.387	1.00	27.23	BBBB
ATOM	4302	CA	GLN	B	229	6.853	-22.046	1.329	1.00	28.38	BBBB
ATOM	4311	CA	ALA	B	230	10.185	-23.754	0.682	1.00	26.18	BBBB
ATOM	4316	CA	TYR	B	231	11.371	-20.766	-1.366	1.00	25.47	BBBB
ATOM	4328	CA	ALA	B	232	10.342	-18.322	1.368	1.00	27.51	BBBB
ATOM	4333	CA	GLU	B	233	12.145	-20.441	3.966	1.00	30.87	BBBB
ATOM	4342	CA	ALA	B	234	15.215	-20.417	1.714	1.00	28.48	BBBB
ATOM	4347	CA	GLY	B	235	15.033	-16.627	1.815	1.00	26.23	BBBB
ATOM	4351	CA	GLN	B	236	14.121	-16.198	-1.870	1.00	25.53	BBBB
ATOM	4361	CA	PRO	B	237	10.336	-15.587	-1.720	1.00	24.65	BBBB
ATOM	4367	CA	GLN	B	238	10.277	-13.558	-4.945	1.00	24.29	BBBB
ATOM	4376	CA	HIS	B	239	10.526	-16.608	-7.201	1.00	22.08	BBBB
ATOM	4386	CA	LYS	B	240	7.375	-17.589	-9.105	1.00	23.26	BBBB
ATOM	4395	CA	VAL	B	241	5.740	-20.911	-8.277	1.00	23.78	BBBB
ATOM	4402	CA	THR	B	242	2.758	-22.301	-10.177	1.00	25.93	BBBB
ATOM	4409	CA	GLU	B	243	0.999	-25.651	-9.837	1.00	27.03	BBBB
ATOM	4418	CA	PHE	B	244	0.964	-26.068	-13.620	1.00	26.54	BBBB
ATOM	4429	CA	ILE	B	245	1.932	-24.242	-16.802	1.00	28.48	BBBB
ATOM	4437	CA	ASP	B	246	-0.754	-24.396	-19.457	1.00	36.00	BBBB
ATOM	4445	CA	ASP	B	247	1.245	-22.392	-21.999	1.00	30.74	BBBB
ATOM	4453	CA	MET	B	248	4.625	-24.136	-22.138	1.00	28.41	BBBB
ATOM	4461	CA	ALA	B	249	5.512	-22.216	-25.290	1.00	24.67	BBBB
ATOM	4466	CA	ALA	B	250	5.188	-18.933	-23.390	1.00	21.78	BBBB
ATOM	4471	CA	ALA	B	251	7.301	-20.259	-20.501	1.00	20.85	BBBB
ATOM	4476	CA	TYR	B	252	9.972	-21.616	-22.886	1.00	22.78	BBBB
ATOM	4488	CA	ALA	B	253	10.131	-18.224	-24.636	1.00	23.54	BBBB
ATOM	4493	CA	TRP	B	254	10.829	-16.534	-21.303	1.00	19.76	BBBB
ATOM	4507	CA	ALA	B	255	13.399	-19.025	-20.003	1.00	19.51	BBBB
ATOM	4512	CA	ASP	B	256	17.176	-19.026	-20.434	1.00	17.58	BBBB
ATOM	4520	CA	VAL	B	257	17.535	-22.603	-19.194	1.00	18.53	BBBB
ATOM	4527	CA	VAL	B	258	15.208	-25.456	-18.234	1.00	19.32	BBBB
ATOM	4534	CA	VAL	B	259	15.581	-27.957	-15.374	1.00	19.85	BBBB
ATOM	4541	CA	CYS	B	260	13.454	-31.055	-15.946	1.00	22.00	BBBB
ATOM	4547	CA	ARG	B	261	13.170	-34.800	-16.515	1.00	23.75	BBBB
ATOM	4558	CA	SER	B	262	13.975	-36.189	-19.948	1.00	23.18	BBBB
ATOM	4564	CA	GLY	B	263	11.026	-38.079	-21.361	1.00	22.85	BBBB
ATOM	4568	CA	ALA	B	264	11.482	-38.564	-25.115	1.00	24.25	BBBB
ATOM	4573	CA	LEU	B	265	8.846	-36.037	-26.205	1.00	24.66	BBBB

ATOM	4581	CA	THR	B	266	10.194	-33.557	-23.657	1.00	22.34	BBBB
ATOM	4588	CA	VAL	B	267	13.730	-33.762	-25.023	1.00	21.11	BBBB
ATOM	4595	CA	SER	B	268	12.411	-33.191	-28.567	1.00	21.96	BBBB
ATOM	4601	CA	GLU	B	269	10.282	-30.272	-27.378	1.00	21.95	BBBB
ATOM	4610	CA	ILE	B	270	13.295	-28.698	-25.638	1.00	20.62	BBBB
ATOM	4618	CA	ALA	B	271	15.440	-29.058	-28.776	1.00	22.45	BBBB
ATOM	4623	CA	ALA	B	272	12.719	-27.451	-30.898	1.00	22.17	BBBB
ATOM	4628	CA	ALA	B	273	12.361	-24.596	-28.407	1.00	21.97	BBBB
ATOM	4633	CA	GLY	B	274	16.093	-24.023	-28.709	1.00	21.07	BBBB
ATOM	4637	CA	LEU	B	275	16.666	-24.057	-24.966	1.00	19.78	BBBB
ATOM	4646	CA	PRO	B	276	19.651	-25.199	-22.875	1.00	16.62	BBBB
ATOM	4652	CA	ALA	B	277	18.638	-27.807	-20.321	1.00	15.80	BBBB
ATOM	4657	CA	LEU	B	278	19.896	-29.429	-17.145	1.00	18.48	BBBB
ATOM	4665	CA	PHE	B	279	18.266	-32.838	-17.392	1.00	21.59	BBBB
ATOM	4676	CA	VAL	B	280	17.502	-34.902	-14.281	1.00	25.67	BBBB
ATOM	4684	CA	PRO	B	281	16.698	-38.320	-15.824	1.00	29.05	BBBB
ATOM	4690	CA	PHE	B	282	14.246	-40.496	-13.926	1.00	37.13	BBBB
ATOM	4701	CA	GLN	B	283	16.319	-43.395	-12.591	1.00	41.11	BBBB
ATOM	4710	CA	HIS	B	284	15.641	-46.917	-13.843	1.00	43.69	BBBB
ATOM	4720	CA	LYS	B	285	17.767	-49.993	-14.571	1.00	45.34	BBBB
ATOM	4729	CA	ASP	B	286	16.949	-49.299	-18.222	1.00	43.26	BBBB
ATOM	4737	CA	ARG	B	287	17.951	-45.623	-17.883	1.00	36.28	BBBB
ATOM	4748	CA	GLN	B	288	15.622	-44.804	-20.755	1.00	30.77	BBBB
ATOM	4757	CA	GLN	B	289	15.474	-41.099	-19.904	1.00	29.46	BBBB
ATOM	4766	CA	TYR	B	290	19.228	-40.984	-19.550	1.00	29.55	BBBB
ATOM	4778	CA	TRP	B	291	19.542	-42.282	-23.116	1.00	28.07	BBBB
ATOM	4792	CA	ASN	B	292	16.902	-39.784	-24.270	1.00	26.06	BBBB
ATOM	4800	CA	ALA	B	293	18.926	-36.822	-22.979	1.00	25.69	BBBB
ATOM	4805	CA	LEU	B	294	22.354	-38.088	-24.032	1.00	25.90	BBBB
ATOM	4814	CA	PRO	B	295	21.998	-36.870	-27.635	1.00	26.15	BBBB
ATOM	4820	CA	LEU	B	296	21.521	-33.265	-26.481	1.00	25.42	BBBB
ATOM	4828	CA	GLU	B	297	24.354	-33.530	-23.953	1.00	28.78	BBBB
ATOM	4837	CA	LYS	B	298	26.644	-34.947	-26.648	1.00	31.90	BBBB
ATOM	4846	CA	ALA	B	299	25.773	-31.965	-28.847	1.00	30.38	BBBB
ATOM	4851	CA	GLY	B	300	26.777	-29.635	-26.017	1.00	26.18	BBBB
ATOM	4855	CA	ALA	B	301	23.214	-28.333	-25.638	1.00	22.50	BBBB
ATOM	4860	CA	ALA	B	302	22.516	-29.770	-22.186	1.00	21.78	BBBB
ATOM	4865	CA	LYS	B	303	23.979	-31.340	-19.048	1.00	25.86	BBBB
ATOM	4874	CA	ILE	B	304	22.753	-34.598	-17.550	1.00	27.17	BBBB
ATOM	4882	CA	ILE	B	305	22.843	-35.178	-13.813	1.00	29.01	BBBB
ATOM	4890	CA	GLU	B	306	21.664	-38.702	-13.061	1.00	34.65	BBBB
ATOM	4899	CA	GLN	B	307	20.377	-39.599	-9.613	1.00	40.54	BBBB
ATOM	4909	CA	PRO	B	308	23.828	-40.891	-8.484	1.00	43.20	BBBB
ATOM	4915	CA	GLN	B	309	25.247	-37.361	-8.787	1.00	43.46	BBBB
ATOM	4924	CA	LEU	B	310	22.232	-35.166	-8.022	1.00	39.65	BBBB
ATOM	4932	CA	SER	B	311	22.660	-32.714	-5.154	1.00	34.90	BBBB
ATOM	4938	CA	VAL	B	312	21.990	-29.074	-4.341	1.00	31.50	BBBB
ATOM	4945	CA	ASP	B	313	25.642	-28.202	-4.957	1.00	29.61	BBBB
ATOM	4953	CA	ALA	B	314	25.782	-30.099	-8.254	1.00	26.47	BBBB
ATOM	4958	CA	VAL	B	315	22.755	-28.215	-9.612	1.00	25.33	BBBB
ATOM	4965	CA	ALA	B	316	23.888	-24.872	-8.199	1.00	27.13	BBBB
ATOM	4970	CA	ASN	B	317	27.444	-25.246	-9.518	1.00	28.52	BBBB
ATOM	4978	CA	THR	B	318	26.174	-26.371	-12.906	1.00	27.04	BBBB
ATOM	4985	CA	LEU	B	319	23.883	-23.370	-13.357	1.00	25.21	BBBB
ATOM	4993	CA	ALA	B	320	26.445	-20.931	-11.957	1.00	24.59	BBBB
ATOM	4998	CA	GLY	B	321	28.934	-22.031	-14.591	1.00	24.34	BBBB
ATOM	5002	CA	TRP	B	322	26.738	-21.007	-17.521	1.00	21.72	BBBB
ATOM	5016	CA	SER	B	323	27.141	-17.404	-18.692	1.00	19.04	BBBB
ATOM	5022	CA	ARG	B	324	24.725	-15.741	-21.112	1.00	18.09	BBBB
ATOM	5033	CA	GLU	B	325	27.220	-16.368	-23.954	1.00	16.96	BBBB
ATOM	5042	CA	THR	B	326	27.460	-20.055	-23.070	1.00	16.39	BBBB
ATOM	5049	CA	LEU	B	327	23.659	-20.305	-22.780	1.00	17.27	BBBB
ATOM	5057	CA	LEU	B	328	23.175	-18.745	-26.222	1.00	17.39	BBBB
ATOM	5065	CA	THR	B	329	25.567	-21.335	-27.688	1.00	21.30	BBBB
ATOM	5072	CA	MET	B	330	23.771	-24.153	-25.870	1.00	19.91	BBBB
ATOM	5080	CA	ALA	B	331	20.412	-22.871	-27.098	1.00	18.49	BBBB

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ATOM   5085  CA  GLU B 332      21.626 -22.827 -30.704  1.00 21.47 BBBB
ATOM   5094  CA  ARG B 333      23.040 -26.330 -30.408  1.00 23.77 BBBB
ATOM   5105  CA  ALA B 334      19.648 -27.420 -29.063  1.00 22.88 BBBB
ATOM   5110  CA  ARG B 335      17.795 -25.892 -32.002  1.00 23.54 BBBB
ATOM   5121  CA  ALA B 336      20.330 -27.477 -34.372  1.00 26.85 BBBB
ATOM   5126  CA  ALA B 337      19.740 -30.925 -32.865  1.00 30.89 BBBB
ATOM   5131  CA  SER B 338      16.008 -30.432 -33.408  1.00 32.41 BBBB
ATOM   5137  CA  ILE B 339      13.882 -31.941 -36.187  1.00 34.35 BBBB
ATOM   5146  CA  PRO B 340      10.733 -29.730 -36.600  1.00 34.94 BBBB
ATOM   5152  CA  ASP B 341       8.711 -31.820 -39.056  1.00 33.33 BBBB
ATOM   5160  CA  ALA B 342       8.875 -35.238 -37.411  1.00 29.09 BBBB
ATOM   5165  CA  THR B 343       5.115 -35.696 -37.744  1.00 28.55 BBBB
ATOM   5172  CA  GLU B 344       5.085 -34.933 -41.480  1.00 32.00 BBBB
ATOM   5181  CA  ARG B 345       8.138 -37.123 -42.067  1.00 31.44 BBBB
ATOM   5192  CA  VAL B 346       6.578 -40.151 -40.384  1.00 28.61 BBBB
ATOM   5199  CA  ALA B 347       3.249 -39.617 -42.137  1.00 28.96 BBBB
ATOM   5204  CA  ASN B 348       5.035 -39.286 -45.493  1.00 34.56 BBBB
ATOM   5212  CA  GLU B 349       6.954 -42.540 -44.956  1.00 34.86 BBBB
ATOM   5221  CA  VAL B 350       3.767 -44.306 -43.919  1.00 33.79 BBBB
ATOM   5228  CA  SER B 351       2.196 -42.946 -47.095  1.00 36.67 BBBB
ATOM   5234  CA  ARG B 352       5.114 -44.088 -49.251  1.00 40.03 BBBB
ATOM   5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78 BBBB
ATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24 BBBB
ATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71 BBBB
ATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93 BBBB
ATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81 BBBB
END
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TABLE 3 ATOMIC COORDINATES OF E.COLI MURG C-ALPHA BACKBONE AND CONSERVED AMINO ACID RESIDUES

ATOM	2649	CA	LYS	B	7	-6.512	-45.403	-47.519	1.00	45.28	BBBB
ATOM	2651	CA	ARG	B	8	-6.682	-47.303	-44.240	1.00	38.63	BBBB
ATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00	30.88	BBBB
ATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00	26.66	BBBB
ATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00	23.16	BBBB
ATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	BBBB
ATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00	29.43	BBBB
ATOM	2697	N	GLY	B	14	0.150	-47.934	-27.405	1.00	32.46	BBBB
ATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00	33.82	BBBB
ATOM	2699	C	GLY	B	14	-0.107	-46.595	-25.299	1.00	34.82	BBBB
ATOM	2700	O	GLY	B	14	0.975	-46.040	-25.479	1.00	35.47	BBBB
ATOM	2701	N	GLY	B	15	-0.986	-46.188	-24.385	1.00	35.56	BBBB
ATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00	36.08	BBBB
ATOM	2703	C	GLY	B	15	0.539	-45.254	-22.683	1.00	36.84	BBBB
ATOM	2704	O	GLY	B	15	1.293	-44.311	-22.426	1.00	36.03	BBBB
ATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00	38.51	BBBB
ATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00	36.57	BBBB
ATOM	2716	N	GLY	B	18	3.949	-43.752	-23.150	1.00	33.83	BBBB
ATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00	33.48	BBBB
ATOM	2718	C	GLY	B	18	3.825	-42.593	-25.378	1.00	33.12	BBBB
ATOM	2719	O	GLY	B	18	4.345	-41.650	-25.984	1.00	35.38	BBBB
ATOM	2720	N	HIS	B	19	3.416	-43.699	-25.988	1.00	30.26	BBBB
ATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00	28.22	BBBB
ATOM	2722	CB	HIS	B	19	3.772	-45.349	-27.779	1.00	25.81	BBBB
ATOM	2723	CG	HIS	B	19	4.957	-45.966	-27.094	1.00	25.35	BBBB
ATOM	2724	CD2	HIS	B	19	6.281	-45.694	-27.184	1.00	24.18	BBBB
ATOM	2725	ND1	HIS	B	19	4.845	-47.025	-26.217	1.00	24.57	BBBB
ATOM	2726	CE1	HIS	B	19	6.046	-47.380	-25.798	1.00	23.08	BBBB
ATOM	2727	NE2	HIS	B	19	6.936	-46.589	-26.369	1.00	25.51	BBBB
ATOM	2728	C	HIS	B	19	2.280	-43.370	-28.144	1.00	27.91	BBBB
ATOM	2729	O	HIS	B	19	2.300	-43.049	-29.337	1.00	26.91	BBBB
ATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00	27.77	BBBB
ATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00	29.00	BBBB
ATOM	2750	CA	PRO	B	22	2.986	-39.252	-31.086	1.00	26.12	BBBB
ATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00	25.07	BBBB
ATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00	25.32	BBBB
ATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00	25.94	BBBB
ATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00	25.70	BBBB
ATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00	26.15	BBBB
ATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00	29.32	BBBB
ATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00	32.38	BBBB
ATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00	32.00	BBBB
ATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00	34.91	BBBB
ATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00	37.55	BBBB
ATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00	38.24	BBBB
ATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00	35.75	BBBB
ATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00	34.58	BBBB
ATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00	35.40	BBBB
ATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00	34.16	BBBB
ATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00	31.56	BBBB
ATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00	27.41	BBBB
ATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71	BBBB
ATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00	23.47	BBBB
ATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00	29.84	BBBB
ATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00	38.81	BBBB
ATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00	44.47	BBBB
ATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00	40.44	BBBB
ATOM	2937	CA	MET	B	46	-4.881	-45.581	-21.249	1.00	36.33	BBBB
ATOM	2945	CA	GLU	B	47	-5.458	-45.655	-25.029	1.00	31.79	BBBB
ATOM	2954	CA	ALA	B	48	-8.821	-47.344	-24.414	1.00	32.58	BBBB
ATOM	2959	CA	ASP	B	49	-10.143	-44.065	-23.009	1.00	35.60	BBBB

ATOM	2967	CA	LEU	B	50	-8.026	-41.484	-24.840	1.00	33.49	BBBB
ATOM	2975	CA	VAL	B	51	-8.299	-42.641	-28.449	1.00	32.68	BBBB
ATOM	2983	CA	PRO	B	52	-12.111	-42.601	-28.453	1.00	34.43	BBBB
ATOM	2989	CA	LYS	B	53	-11.998	-39.054	-27.064	1.00	36.73	BBBB
ATOM	2998	CA	HIS	B	54	-10.116	-38.212	-30.259	1.00	34.62	BBBB
ATOM	3008	CA	GLY	B	55	-12.938	-39.481	-32.447	1.00	35.34	BBBB
ATOM	3012	CA	ILE	B	56	-10.909	-42.517	-33.514	1.00	33.81	BBBB
ATOM	3020	CA	GLU	B	57	-12.228	-46.083	-33.467	1.00	34.16	BBBB
ATOM	3029	CA	ILE	B	58	-10.217	-48.658	-31.553	1.00	31.38	BBBB
ATOM	3037	CA	ASP	B	59	-10.039	-52.442	-31.720	1.00	31.09	BBBB
ATOM	3045	CA	PHE	B	60	-8.809	-54.410	-28.713	1.00	30.32	BBBB
ATOM	3056	CA	ILE	B	61	-6.832	-57.616	-28.269	1.00	28.55	BBBB
ATOM	3064	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00	30.76	BBBB
ATOM	3075	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	BBBB
ATOM	3083	CA	SER	B	64	-2.356	-60.520	-20.505	1.00	37.51	BBBB
ATOM	3089	CA	GLY	B	65	0.679	-62.355	-19.199	1.00	37.13	BBBB
ATOM	3093	CA	LEU	B	66	2.591	-61.413	-22.355	1.00	33.17	BBBB
ATOM	3101	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	BBBB
ATOM	3112	CA	GLY	B	68	7.380	-57.427	-20.685	1.00	26.79	BBBB
ATOM	3116	CA	LYS	B	69	8.238	-60.463	-22.796	1.00	23.93	BBBB
ATOM	3125	CA	GLY	B	70	10.755	-60.229	-25.636	1.00	22.26	BBBB
ATOM	3129	CA	ILE	B	71	10.357	-62.386	-28.762	1.00	23.55	BBBB
ATOM	3137	CA	LYS	B	72	12.038	-65.491	-27.343	1.00	24.92	BBBB
ATOM	3146	CA	ALA	B	73	9.839	-65.306	-24.233	1.00	21.18	BBBB
ATOM	3151	CA	LEU	B	74	6.745	-64.762	-26.387	1.00	19.36	BBBB
ATOM	3159	CA	ILE	B	75	7.434	-67.768	-28.601	1.00	21.18	BBBB
ATOM	3167	CA	ALA	B	76	7.996	-69.726	-25.374	1.00	21.72	BBBB
ATOM	3172	CA	ALA	B	77	4.289	-69.121	-24.655	1.00	21.07	BBBB
ATOM	3178	CA	PRO	B	78	2.772	-70.846	-27.771	1.00	20.95	BBBB
ATOM	3184	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00	21.32	BBBB
ATOM	3192	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00	21.30	BBBB
ATOM	3203	CA	ILE	B	81	1.113	-65.621	-28.421	1.00	19.47	BBBB
ATOM	3211	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00	19.15	BBBB
ATOM	3222	CA	ASN	B	83	-4.150	-66.332	-29.577	1.00	20.90	BBBB
ATOM	3230	CA	ALA	B	84	-3.177	-62.647	-29.484	1.00	19.30	BBBB
ATOM	3235	CA	TRP	B	85	-1.820	-63.111	-33.032	1.00	20.56	BBBB
ATOM	3249	CA	ARG	B	86	-5.140	-64.660	-34.166	1.00	23.28	BBBB
ATOM	3260	CA	GLN	B	87	-7.101	-61.802	-32.567	1.00	24.07	BBBB
ATOM	3269	CA	ALA	B	88	-4.996	-59.183	-34.355	1.00	23.78	BBBB
ATOM	3274	CA	ARG	B	89	-5.285	-61.111	-37.636	1.00	24.94	BBBB
ATOM	3285	CA	ALA	B	90	-9.088	-61.151	-37.383	1.00	26.16	BBBB
ATOM	3290	CA	ILE	B	91	-9.108	-57.400	-36.733	1.00	26.97	BBBB
ATOM	3298	CA	MET	B	92	-6.872	-56.693	-39.717	1.00	29.03	BBBB
ATOM	3306	CA	LYS	B	93	-8.735	-59.038	-42.050	1.00	33.20	BBBB
ATOM	3315	CA	ALA	B	94	-11.943	-57.157	-41.183	1.00	33.62	BBBB
ATOM	3320	CA	TYR	B	95	-10.504	-53.620	-41.224	1.00	33.83	BBBB
ATOM	3332	CA	LYS	B	96	-8.104	-54.327	-44.122	1.00	33.85	BBBB
ATOM	3342	CA	PRO	B	97	-5.490	-51.623	-43.419	1.00	31.82	BBBB
ATOM	3348	CA	ASP	B	98	-3.049	-50.685	-46.188	1.00	29.78	BBBB
ATOM	3356	CA	VAL	B	99	-0.296	-50.214	-43.660	1.00	26.75	BBBB
ATOM	3363	CA	VAL	B	100	0.227	-50.613	-39.936	1.00	23.59	BBBB
ATOM	3370	CA	LEU	B	101	2.214	-48.199	-37.797	1.00	21.59	BBBB
ATOM	3378	CA	GLY	B	102	3.796	-49.357	-34.549	1.00	19.23	BBBB
ATOM	3382	CA	MET	B	103	4.892	-46.597	-32.191	1.00	18.93	BBBB
ATOM	3389	N	GLY	B	104	5.640	-48.450	-30.827	1.00	21.56	BBBB
ATOM	3390	CA	GLY	B	104	6.275	-49.080	-29.686	1.00	21.89	BBBB
ATOM	3391	C	GLY	B	104	5.192	-49.614	-28.764	1.00	23.28	BBBB
ATOM	3392	O	GLY	B	104	4.009	-49.353	-28.980	1.00	22.50	BBBB
ATOM	3394	CA	GLY	B	105	4.593	-50.905	-26.827	1.00	23.54	BBBB
ATOM	3398	CA	TYR	B	106	3.818	-54.554	-26.159	1.00	22.37	BBBB
ATOM	3410	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06	BBBB
ATOM	3417	CA	SER	B	108	2.488	-53.892	-31.290	1.00	19.67	BBBB
ATOM	3423	CA	GLY	B	109	4.251	-57.256	-31.023	1.00	20.03	BBBB
ATOM	3428	CA	PRO	B	110	1.251	-59.478	-31.855	1.00	18.99	BBBB
ATOM	3434	CA	GLY	B	111	-0.160	-56.702	-34.025	1.00	19.60	BBBB
ATOM	3438	CA	GLY	B	112	3.014	-56.417	-36.074	1.00	19.97	BBBB

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ATOM   3442  CA  LEU B 113      3.265 -60.184 -36.429  1.00 19.49 BBBB
ATOM   3450  CA  ALA B 114     -0.334 -60.292 -37.661  1.00 18.70 BBBB
ATOM   3455  CA  ALA B 115      0.167 -57.516 -40.229  1.00 21.84 BBBB
ATOM   3460  CA  TRP B 116      3.365 -59.126 -41.478  1.00 23.22 BBBB
ATOM   3474  CA  SER B 117      1.735 -62.573 -41.873  1.00 22.61 BBBB
ATOM   3480  CA  LEU B 118     -1.069 -60.957 -43.882  1.00 25.70 BBBB
ATOM   3488  CA  GLY B 119      1.354 -59.174 -46.192  1.00 27.80 BBBB
ATOM   3492  CA  ILE B 120      0.568 -55.744 -44.731  1.00 24.85 BBBB
ATOM   3501  CA  PRO B 121      3.625 -53.477 -44.591  1.00 22.63 BBBB
ATOM   3507  CA  VAL B 122      4.743 -52.594 -41.083  1.00 22.03 BBBB
ATOM   3514  CA  VAL B 123      6.200 -49.184 -40.310  1.00 20.82 BBBB
ATOM   3521  CA  LEU B 124      7.749 -48.485 -36.915  1.00 22.10 BBBB
ATOM   3528  N   HIS B 125      8.182 -46.638 -35.447  1.00 21.40 BBBB
ATOM   3529  CA  HIS B 125      8.814 -45.413 -34.981  1.00 21.42 BBBB
ATOM   3530  CB  HIS B 125      7.858 -44.218 -35.067  1.00 21.57 BBBB
ATOM   3531  CG  HIS B 125      8.432 -42.948 -34.511  1.00 23.73 BBBB
ATOM   3532  CD2 HIS B 125      8.300 -42.368 -33.295  1.00 22.15 BBBB
ATOM   3533  ND1 HIS B 125      9.274 -42.127 -35.236  1.00 26.23 BBBB
ATOM   3534  CE1 HIS B 125      9.631 -41.095 -34.490  1.00 24.20 BBBB
ATOM   3535  NE2 HIS B 125      9.054 -41.218 -33.307  1.00 26.07 BBBB
ATOM   3536  C   HIS B 125      9.196 -45.642 -33.519  1.00 21.70 BBBB
ATOM   3537  O   HIS B 125      8.378 -46.117 -32.725  1.00 19.81 BBBB
ATOM   3538  N   GLU B 126     10.444 -45.332 -33.186  1.00 21.20 BBBB
ATOM   3539  CA  GLU B 126     10.947 -45.452 -31.817  1.00 22.15 BBBB
ATOM   3540  CB  GLU B 126     12.252 -46.246 -31.790  1.00 21.99 BBBB
ATOM   3541  CG  GLU B 126     12.958 -46.206 -30.439  1.00 22.04 BBBB
ATOM   3542  CD  GLU B 126     12.119 -46.824 -29.338  1.00 21.43 BBBB
ATOM   3543  OE1 GLU B 126     11.767 -48.014 -29.471  1.00 21.92 BBBB
ATOM   3544  OE2 GLU B 126     11.807 -46.124 -28.349  1.00 21.08 BBBB
ATOM   3545  C   GLU B 126     11.205 -44.027 -31.326  1.00 21.93 BBBB
ATOM   3546  O   GLU B 126     12.016 -43.300 -31.908  1.00 21.33 BBBB
ATOM   3548  CA  GLN B 127     10.682 -42.270 -29.735  1.00 22.81 BBBB
ATOM   3557  CA  ASN B 128     13.406 -43.097 -27.216  1.00 22.96 BBBB
ATOM   3565  CA  GLY B 129     17.203 -43.019 -27.294  1.00 25.36 BBBB
ATOM   3569  CA  ILE B 130     17.160 -46.716 -26.488  1.00 28.00 BBBB
ATOM   3577  CA  ALA B 131     14.978 -49.139 -28.461  1.00 25.88 BBBB
ATOM   3582  CA  GLY B 132     12.007 -50.532 -26.568  1.00 24.05 BBBB
ATOM   3586  CA  LEU B 133     11.903 -54.293 -26.020  1.00 24.54 BBBB
ATOM   3594  CA  THR B 134      9.202 -54.860 -28.639  1.00 21.22 BBBB
ATOM   3601  CA  ASN B 135     10.407 -52.419 -31.324  1.00 20.50 BBBB
ATOM   3609  CA  LYS B 136     13.886 -53.949 -31.144  1.00 22.79 BBBB
ATOM   3618  CA  TRP B 137     12.753 -57.345 -32.424  1.00 22.06 BBBB
ATOM   3632  CA  LEU B 138      9.744 -56.188 -34.431  1.00 23.15 BBBB
ATOM   3640  CA  ALA B 139     12.128 -54.092 -36.542  1.00 25.29 BBBB
ATOM   3645  CA  LYS B 140     13.279 -57.337 -38.182  1.00 28.05 BBBB
ATOM   3654  CA  ILE B 141      9.963 -57.818 -40.016  1.00 26.09 BBBB
ATOM   3662  CA  ALA B 142      9.331 -54.107 -40.498  1.00 25.03 BBBB
ATOM   3667  CA  THR B 143      9.262 -52.595 -43.984  1.00 26.10 BBBB
ATOM   3674  CA  LYS B 144     10.436 -49.238 -42.618  1.00 24.73 BBBB
ATOM   3683  CA  VAL B 145     11.947 -48.311 -39.252  1.00 23.62 BBBB
ATOM   3690  CA  MET B 146     12.338 -44.736 -37.993  1.00 23.15 BBBB
ATOM   3698  CA  GLN B 147     13.762 -43.418 -34.712  1.00 25.05 BBBB
ATOM   3707  CA  ALA B 148     13.559 -40.032 -33.009  1.00 26.88 BBBB
ATOM   3712  CA  PHE B 149     17.239 -39.820 -32.098  1.00 29.39 BBBB
ATOM   3724  CA  PRO B 150     20.310 -41.541 -33.535  1.00 31.87 BBBB
ATOM   3730  CA  GLY B 151     21.629 -44.537 -31.595  1.00 32.62 BBBB
ATOM   3734  CA  ALA B 152     18.447 -46.476 -30.753  1.00 32.71 BBBB
ATOM   3739  CA  PHE B 153     18.925 -48.506 -33.937  1.00 34.83 BBBB
ATOM   3751  CA  PRO B 154     22.158 -48.751 -35.993  1.00 38.97 BBBB
ATOM   3757  CA  ASN B 155     20.765 -47.568 -39.346  1.00 41.08 BBBB
ATOM   3765  CA  ALA B 156     17.170 -46.407 -38.843  1.00 37.55 BBBB
ATOM   3770  CA  GLU B 157     16.367 -43.044 -40.460  1.00 34.40 BBBB
ATOM   3779  CA  VAL B 158     16.337 -40.344 -37.764  1.00 31.16 BBBB
ATOM   3786  CA  VAL B 159     13.155 -38.265 -37.889  1.00 28.10 BBBB
ATOM   3793  CA  GLY B 160     12.724 -36.921 -34.355  1.00 26.93 BBBB
ATOM   3797  CA  ASN B 161      9.456 -36.807 -32.375  1.00 25.27 BBBB
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ATOM   3806  CA  PRO B 162       6.315 -34.747 -33.004  1.00 26.14 BBBB
ATOM   3812  CA  VAL B 163       6.456 -31.379 -31.216  1.00 27.75 BBBB
ATOM   3819  CA  ARG B 164       3.667 -28.953 -30.246  1.00 32.36 BBBB
ATOM   3830  CA  THR B 165       3.038 -26.307 -32.924  1.00 31.74 BBBB
ATOM   3837  CA  ASP B 166       3.252 -23.404 -30.466  1.00 30.64 BBBB
ATOM   3845  CA  VAL B 167       6.746 -24.503 -29.440  1.00 25.91 BBBB
ATOM   3852  CA  LEU B 168       7.780 -25.002 -33.075  1.00 28.46 BBBB
ATOM   3860  CA  ALA B 169       6.580 -21.455 -33.756  1.00 31.43 BBBB
ATOM   3865  CA  LEU B 170       9.002 -19.905 -31.268  1.00 29.60 BBBB
ATOM   3874  CA  PRO B 171      11.611 -17.457 -32.642  1.00 30.11 BBBB
ATOM   3880  CA  LEU B 172      15.157 -18.780 -33.062  1.00 28.33 BBBB
ATOM   3889  CA  PRO B 173      17.450 -18.550 -29.977  1.00 25.25 BBBB
ATOM   3895  CA  GLN B 174      19.526 -15.527 -31.049  1.00 25.46 BBBB
ATOM   3904  CA  GLN B 175      16.365 -13.525 -31.718  1.00 28.47 BBBB
ATOM   3913  CA  ARG B 176      14.611 -14.635 -28.525  1.00 29.01 BBBB
ATOM   3924  CA  LEU B 177      17.673 -13.970 -26.331  1.00 29.90 BBBB
ATOM   3932  CA  ALA B 178      18.766 -10.776 -28.131  1.00 30.78 BBBB
ATOM   3937  CA  GLY B 179      19.846  -7.993 -25.784  1.00 30.10 BBBB
ATOM   3941  CA  ARG B 180      18.676  -9.965 -22.787  1.00 28.97 BBBB
ATOM   3952  CA  GLU B 181      20.545  -9.027 -19.621  1.00 31.79 BBBB
ATOM   3961  CA  GLY B 182      19.871  -9.586 -15.943  1.00 27.75 BBBB
ATOM   3966  CA  PRO B 183      19.450 -12.832 -13.913  1.00 22.93 BBBB
ATOM   3972  CA  VAL B 184      19.524 -16.146 -15.729  1.00 18.01 BBBB
ATOM   3979  CA  ARG B 185      15.873 -17.216 -16.011  1.00 17.62 BBBB
ATOM   3990  CA  VAL B 186      15.508 -20.771 -14.741  1.00 16.47 BBBB
ATOM   3997  CA  LEU B 187      12.361 -22.710 -15.604  1.00 16.75 BBBB
ATOM   4005  CA  VAL B 188      11.774 -25.775 -13.381  1.00 18.41 BBBB
ATOM   4012  CA  VAL B 189       9.298 -28.234 -14.948  1.00 22.11 BBBB
ATOM   4018  N   GLY B 190       8.111 -29.887 -13.615  1.00 25.60 BBBB
ATOM   4019  CA  GLY B 190       7.914 -31.188 -12.994  1.00 27.28 BBBB
ATOM   4020  C   GLY B 190       6.808 -32.026 -13.604  1.00 29.67 BBBB
ATOM   4021  O   GLY B 190       6.668 -33.208 -13.283  1.00 29.86 BBBB
ATOM   4022  N   GLY B 191       6.025 -31.430 -14.497  1.00 30.56 BBBB
ATOM   4023  CA  GLY B 191       4.935 -32.163 -15.115  1.00 31.94 BBBB
ATOM   4024  C   GLY B 191       3.676 -32.104 -14.269  1.00 33.11 BBBB
ATOM   4025  O   GLY B 191       3.691 -31.556 -13.165  1.00 32.14 BBBB
ATOM   4026  N   SER B 192       2.587 -32.673 -14.779  1.00 34.23 BBBB
ATOM   4027  CA  SER B 192       1.313 -32.665 -14.064  1.00 35.91 BBBB
ATOM   4028  CB  SER B 192       0.283 -33.532 -14.801  1.00 36.87 BBBB
ATOM   4029  OG  SER B 192       0.702 -34.887 -14.877  1.00 39.58 BBBB
ATOM   4030  C   SER B 192       1.419 -33.128 -12.609  1.00 36.41 BBBB
ATOM   4031  O   SER B 192       0.862 -32.499 -11.714  1.00 35.78 BBBB
ATOM   4033  CA  GLN B 193       2.292 -34.763 -11.033  1.00 38.53 BBBB
ATOM   4041  N   GLY B 194       4.291 -33.398 -10.986  1.00 36.47 BBBB
ATOM   4042  CA  GLY B 194       5.398 -32.711 -10.350  1.00 35.02 BBBB
ATOM   4043  C   GLY B 194       6.584 -33.630 -10.146  1.00 34.51 BBBB
ATOM   4044  O   GLY B 194       6.442 -34.851 -10.191  1.00 34.26 BBBB
ATOM   4045  N   ALA B 195       7.761 -33.045  -9.938  1.00 33.54 BBBB
ATOM   4046  CA  ALA B 195       8.977 -33.819  -9.709  1.00 33.12 BBBB
ATOM   4047  CB  ALA B 195      10.073 -33.387 -10.679  1.00 33.17 BBBB
ATOM   4048  C   ALA B 195       9.423 -33.590  -8.267  1.00 32.87 BBBB
ATOM   4049  O   ALA B 195       9.955 -32.533  -7.923  1.00 31.47 BBBB
ATOM   4051  CA  ARG B 196       9.538 -34.512  -6.010  1.00 32.63 BBBB
ATOM   4062  CA  ILE B 197      13.329 -34.168  -6.164  1.00 28.10 BBBB
ATOM   4070  CA  LEU B 198      13.069 -30.833  -8.003  1.00 26.58 BBBB
ATOM   4078  CA  ASN B 199      10.497 -29.447  -5.563  1.00 27.07 BBBB
ATOM   4086  CA  GLN B 200      12.955 -30.326  -2.794  1.00 30.10 BBBB
ATOM   4095  CA  THR B 201      16.215 -29.345  -4.474  1.00 27.34 BBBB
ATOM   4102  CA  MET B 202      15.567 -26.048  -6.268  1.00 23.68 BBBB
ATOM   4111  CA  PRO B 203      14.608 -23.963  -3.220  1.00 23.84 BBBB
ATOM   4117  CA  GLN B 204      18.033 -24.708  -1.684  1.00 26.34 BBBB
ATOM   4126  CA  VAL B 205      19.672 -24.033  -5.043  1.00 24.44 BBBB
ATOM   4133  CA  ALA B 206      17.980 -20.610  -5.013  1.00 22.84 BBBB
ATOM   4138  CA  ALA B 207      19.442 -19.857  -1.576  1.00 26.65 BBBB
ATOM   4143  CA  LYS B 208      22.915 -20.595  -2.919  1.00 28.31 BBBB
ATOM   4152  CA  LEU B 209      22.577 -18.640  -6.171  1.00 25.68 BBBB
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ATOM   4160  CA  GLY B 210     20.675 -15.628  -4.804  1.00 26.56 BBBB
ATOM   4164  CA  ASP B 211     20.370 -12.647  -7.190  1.00 28.28 BBBB
ATOM   4172  CA  SER B 212     22.098 -14.474 -10.067  1.00 25.73 BBBB
ATOM   4178  CA  VAL B 213     18.925 -16.308 -11.116  1.00 20.76 BBBB
ATOM   4185  CA  THR B 214     15.204 -15.726 -11.337  1.00 19.60 BBBB
ATOM   4192  CA  ILE B 215     13.076 -18.850 -11.169  1.00 18.75 BBBB
ATOM   4200  CA  TRP B 216      9.661 -19.973 -12.378  1.00 19.34 BBBB
ATOM   4214  CA  HIS B 217      9.015 -23.303 -10.680  1.00 21.06 BBBB
ATOM   4224  CA  GLN B 218      6.149 -25.594 -11.735  1.00 24.30 BBBB
ATOM   4233  CA  SER B 219      5.463 -27.800  -8.684  1.00 26.73 BBBB
ATOM   4239  CA  GLY B 220      2.855 -30.242  -9.961  1.00 30.53 BBBB
ATOM   4243  CA  LYS B 221     -0.657 -30.914  -8.628  1.00 35.12 BBBB
ATOM   4252  CA  GLY B 222     -1.195 -29.899  -5.011  1.00 35.34 BBBB
ATOM   4256  CA  SER B 223      2.451 -28.934  -4.418  1.00 33.98 BBBB
ATOM   4262  CA  GLN B 224      2.187 -25.208  -5.186  1.00 33.71 BBBB
ATOM   4271  CA  GLN B 225      1.823 -24.239  -1.519  1.00 32.32 BBBB
ATOM   4280  CA  SER B 226      4.701 -26.309  -0.122  1.00 28.30 BBBB
ATOM   4286  CA  VAL B 227      7.214 -25.247  -2.791  1.00 24.28 BBBB
ATOM   4293  CA  GLU B 228      6.178 -21.592  -2.387  1.00 27.23 BBBB
ATOM   4302  CA  GLN B 229      6.853 -22.046   1.329  1.00 28.38 BBBB
ATOM   4311  CA  ALA B 230     10.185 -23.754   0.682  1.00 26.18 BBBB
ATOM   4316  CA  TYR B 231     11.371 -20.766  -1.366  1.00 25.47 BBBB
ATOM   4328  CA  ALA B 232     10.342 -18.322   1.368  1.00 27.51 BBBB
ATOM   4333  CA  GLU B 233     12.145 -20.441   3.966  1.00 30.87 BBBB
ATOM   4342  CA  ALA B 234     15.215 -20.417   1.714  1.00 28.48 BBBB
ATOM   4347  CA  GLY B 235     15.033 -16.627   1.815  1.00 26.23 BBBB
ATOM   4351  CA  GLN B 236     14.121 -16.198  -1.870  1.00 25.53 BBBB
ATOM   4361  CA  PRO B 237     10.336 -15.587  -1.720  1.00 24.65 BBBB
ATOM   4367  CA  GLN B 238     10.277 -13.558  -4.945  1.00 24.29 BBBB
ATOM   4376  CA  HIS B 239     10.526 -16.608  -7.201  1.00 22.08 BBBB
ATOM   4386  CA  LYS B 240      7.375 -17.589  -9.105  1.00 23.26 BBBB
ATOM   4395  CA  VAL B 241      5.740 -20.911  -8.277  1.00 23.78 BBBB
ATOM   4402  CA  THR B 242      2.758 -22.301 -10.177  1.00 25.93 BBBB
ATOM   4409  CA  GLU B 243      0.999 -25.651  -9.837  1.00 27.03 BBBB
ATOM   4418  CA  PHE B 244      0.964 -26.068 -13.620  1.00 26.54 BBBB
ATOM   4429  CA  ILE B 245      1.932 -24.242 -16.802  1.00 28.48 BBBB
ATOM   4437  CA  ASP B 246     -0.754 -24.396 -19.457  1.00 36.00 BBBB
ATOM   4445  CA  ASP B 247      1.245 -22.392 -21.999  1.00 30.74 BBBB
ATOM   4453  CA  MET B 248      4.625 -24.136 -22.138  1.00 28.41 BBBB
ATOM   4461  CA  ALA B 249      5.512 -22.216 -25.290  1.00 24.67 BBBB
ATOM   4466  CA  ALA B 250      5.188 -18.933 -23.390  1.00 21.78 BBBB
ATOM   4471  CA  ALA B 251      7.301 -20.259 -20.501  1.00 20.85 BBBB
ATOM   4476  CA  TYR B 252      9.972 -21.616 -22.886  1.00 22.78 BBBB
ATOM   4488  CA  ALA B 253     10.131 -18.224 -24.636  1.00 23.54 BBBB
ATOM   4493  CA  TRP B 254     10.829 -16.534 -21.303  1.00 19.76 BBBB
ATOM   4507  CA  ALA B 255     13.399 -19.025 -20.003  1.00 19.51 BBBB
ATOM   4512  CA  ASP B 256     17.176 -19.026 -20.434  1.00 17.58 BBBB
ATOM   4520  CA  VAL B 257     17.535 -22.603 -19.194  1.00 18.53 BBBB
ATOM   4527  CA  VAL B 258     15.208 -25.456 -18.234  1.00 19.32 BBBB
ATOM   4534  CA  VAL B 259     15.581 -27.957 -15.374  1.00 19.85 BBBB
ATOM   4541  CA  CYS B 260     13.454 -31.055 -15.946  1.00 22.00 BBBB
ATOM   4546  N   ARG B 261     12.937 -33.397 -16.212  1.00 22.34 BBBB
ATOM   4547  CA  ARG B 261     13.170 -34.800 -16.515  1.00 23.75 BBBB
ATOM   4548  CB  ARG B 261     11.964 -35.663 -16.104  1.00 27.16 BBBB
ATOM   4549  CG  ARG B 261     11.376 -35.337 -14.738  1.00 31.82 BBBB
ATOM   4550  CD  ARG B 261     11.490 -36.473 -13.732  1.00 36.33 BBBB
ATOM   4551  NE  ARG B 261     12.865 -36.721 -13.323  1.00 38.48 BBBB
ATOM   4552  CZ  ARG B 261     13.218 -37.176 -12.125  1.00 37.25 BBBB
ATOM   4553  NH1 ARG B 261     12.295 -37.433 -11.204  1.00 38.46 BBBB
ATOM   4554  NH2 ARG B 261     14.499 -37.370 -11.848  1.00 36.79 BBBB
ATOM   4555  C   ARG B 261     13.351 -34.871 -18.032  1.00 23.98 BBBB
ATOM   4556  O   ARG B 261     13.117 -33.883 -18.746  1.00 22.44 BBBB
ATOM   4558  CA  SER B 262     13.975 -36.189 -19.948  1.00 23.18 BBBB
ATOM   4563  N   GLY B 263     11.850 -37.151 -20.619  1.00 22.74 BBBB
ATOM   4564  CA  GLY B 263     11.026 -38.079 -21.361  1.00 22.85 BBBB
ATOM   4565  C   GLY B 263     11.392 -37.793 -22.813  1.00 24.06 BBBB
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ATOM   4566  O   GLY B 263      11.908 -36.705 -23.121  1.00 22.75 BBBB
ATOM   4567  N   ALA B 264      11.130 -38.739 -23.708  1.00 23.37 BBBB
ATOM   4568  CA  ALA B 264      11.482 -38.564 -25.115  1.00 24.25 BBBB
ATOM   4569  CB  ALA B 264      11.133 -39.829 -25.894  1.00 24.58 BBBB
ATOM   4570  C   ALA B 264      10.843 -37.343 -25.783  1.00 24.29 BBBB
ATOM   4571  O   ALA B 264      11.523 -36.572 -26.470  1.00 24.33 BBBB
ATOM   4573  CA  LEU B 265       8.846 -36.037 -26.205  1.00 24.66 BBBB
ATOM   4581  CA  THR B 266      10.194 -33.557 -23.657  1.00 22.34 BBBB
ATOM   4588  CA  VAL B 267      13.730 -33.762 -25.023  1.00 21.11 BBBB
ATOM   4595  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96 BBBB
ATOM   4600  N   GLU B 269      10.928 -31.563 -27.557  1.00 21.64 BBBB
ATOM   4601  CA  GLU B 269      10.282 -30.272 -27.378  1.00 21.95 BBBB
ATOM   4602  CB  GLU B 269       9.213 -30.399 -26.292  1.00 24.72 BBBB
ATOM   4603  CG  GLU B 269       8.480 -29.128 -25.940  1.00 27.67 BBBB
ATOM   4604  CD  GLU B 269       7.385 -29.380 -24.908  1.00 30.05 BBBB
ATOM   4605  OE1 GLU B 269       6.325 -29.915 -25.287  1.00 31.50 BBBB
ATOM   4606  OE2 GLU B 269       7.591 -29.057 -23.719  1.00 29.84 BBBB
ATOM   4607  C   GLU B 269      11.321 -29.214 -26.999  1.00 21.68 BBBB
ATOM   4608  O   GLU B 269      11.301 -28.095 -27.518  1.00 18.12 BBBB
ATOM   4610  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62 BBBB
ATOM   4618  CA  ALA B 271      15.440 -29.058 -28.776  1.00 22.45 BBBB
ATOM   4623  CA  ALA B 272      12.719 -27.451 -30.898  1.00 22.17 BBBB
ATOM   4628  CA  ALA B 273      12.361 -24.596 -28.407  1.00 21.97 BBBB
ATOM   4633  CA  GLY B 274      16.093 -24.023 -28.709  1.00 21.07 BBBB
ATOM   4637  CA  LEU B 275      16.666 -24.057 -24.966  1.00 19.78 BBBB
ATOM   4646  CA  PRO B 276      19.651 -25.199 -22.875  1.00 16.62 BBBB
ATOM   4652  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80 BBBB
ATOM   4657  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48 BBBB
ATOM   4665  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59 BBBB
ATOM   4676  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67 BBBB
ATOM   4682  N   PRO B 281      17.324 -37.080 -15.370  1.00 27.08 BBBB
ATOM   4683  CD  PRO B 281      18.750 -37.057 -15.726  1.00 27.31 BBBB
ATOM   4684  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05 BBBB
ATOM   4685  CB  PRO B 281      17.851 -39.071 -16.492  1.00 29.44 BBBB
ATOM   4686  CG  PRO B 281      18.791 -37.992 -16.895  1.00 29.67 BBBB
ATOM   4687  C   PRO B 281      16.092 -39.121 -14.684  1.00 31.51 BBBB
ATOM   4688  O   PRO B 281      16.675 -39.223 -13.603  1.00 32.26 BBBB
ATOM   4690  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13 BBBB
ATOM   4701  CA  GLN B 283      16.319 -43.395 -12.591  1.00 41.11 BBBB
ATOM   4710  CA  HIS B 284      15.641 -46.917 -13.843  1.00 43.69 BBBB
ATOM   4720  CA  LYS B 285      17.767 -49.993 -14.571  1.00 45.34 BBBB
ATOM   4729  CA  ASP B 286      16.949 -49.299 -18.222  1.00 43.26 BBBB
ATOM   4737  CA  ARG B 287      17.951 -45.623 -17.883  1.00 36.28 BBBB
ATOM   4748  CA  GLN B 288      15.622 -44.804 -20.755  1.00 30.77 BBBB
ATOM   4756  N   GLN B 289      15.378 -42.554 -19.857  1.00 29.38 BBBB
ATOM   4757  CA  GLN B 289      15.474 -41.099 -19.904  1.00 29.46 BBBB
ATOM   4758  CB  GLN B 289      14.772 -40.472 -18.700  1.00 29.25 BBBB
ATOM   4759  CG  GLN B 289      13.265 -40.416 -18.883  1.00 29.32 BBBB
ATOM   4760  CD  GLN B 289      12.575 -39.585 -17.826  1.00 29.84 BBBB
ATOM   4761  OE1 GLN B 289      13.191 -38.728 -17.188  1.00 29.52 BBBB
ATOM   4762  NE2 GLN B 289      11.281 -39.821 -17.647  1.00 28.95 BBBB
ATOM   4763  C   GLN B 289      16.906 -40.613 -20.005  1.00 29.36 BBBB
ATOM   4764  O   GLN B 289      17.173 -39.557 -20.585  1.00 29.12 BBBB
ATOM   4766  CA  TYR B 290      19.228 -40.984 -19.550  1.00 29.55 BBBB
ATOM   4778  CA  TRP B 291      19.542 -42.282 -23.116  1.00 28.07 BBBB
ATOM   4791  N   ASN B 292      17.658 -40.779 -23.508  1.00 25.52 BBBB
ATOM   4792  CA  ASN B 292      16.902 -39.784 -24.270  1.00 26.06 BBBB
ATOM   4793  CB  ASN B 292      15.484 -39.599 -23.709  1.00 24.78 BBBB
ATOM   4794  CG  ASN B 292      14.590 -40.811 -23.928  1.00 24.46 BBBB
ATOM   4795  OD1 ASN B 292      14.842 -41.641 -24.798  1.00 25.33 BBBB
ATOM   4796  ND2 ASN B 292      13.523 -40.900 -23.146  1.00 23.83 BBBB
ATOM   4797  C   ASN B 292      17.605 -38.427 -24.258  1.00 25.99 BBBB
ATOM   4798  O   ASN B 292      17.566 -37.687 -25.244  1.00 26.18 BBBB
ATOM   4799  N   ALA B 293      18.242 -38.105 -23.139  1.00 25.66 BBBB
ATOM   4800  CA  ALA B 293      18.926 -36.822 -22.979  1.00 25.69 BBBB
ATOM   4801  CB  ALA B 293      18.940 -36.422 -21.506  1.00 24.17 BBBB
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ATOM   4802  C   ALA B 293      20.346 -36.800 -23.521  1.00 25.67 BBBB
ATOM   4803  O   ALA B 293      20.855 -35.743 -23.902  1.00 25.52 BBBB
ATOM   4805  CA  LEU B 294      22.354 -38.088 -24.032  1.00 25.90 BBBB
ATOM   4814  CA  PRO B 295      21.998 -36.870 -27.635  1.00 26.15 BBBB
ATOM   4820  CA  LEU B 296      21.521 -33.265 -26.481  1.00 25.42 BBBB
ATOM   4828  CA  GLU B 297      24.354 -33.530 -23.953  1.00 28.78 BBBB
ATOM   4837  CA  LYS B 298      26.644 -34.947 -26.648  1.00 31.90 BBBB
ATOM   4846  CA  ALA B 299      25.773 -31.965 -28.847  1.00 30.38 BBBB
ATOM   4851  CA  GLY B 300      26.777 -29.635 -26.017  1.00 26.18 BBBB
ATOM   4855  CA  ALA B 301      23.214 -28.333 -25.638  1.00 22.50 BBBB
ATOM   4860  CA  ALA B 302      22.516 -29.770 -22.186  1.00 21.78 BBBB
ATOM   4865  CA  LYS B 303      23.979 -31.340 -19.048  1.00 25.86 BBBB
ATOM   4874  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17 BBBB
ATOM   4882  CA  ILE B 305      22.843 -35.178 -13.813  1.00 29.01 BBBB
ATOM   4890  CA  GLU B 306      21.664 -38.702 -13.061  1.00 34.65 BBBB
ATOM   4899  CA  GLN B 307      20.377 -39.599  -9.613  1.00 40.54 BBBB
ATOM   4909  CA  PRO B 308      23.828 -40.891  -8.484  1.00 43.20 BBBB
ATOM   4915  CA  GLN B 309      25.247 -37.361  -8.787  1.00 43.46 BBBB
ATOM   4924  CA  LEU B 310      22.232 -35.166  -8.022  1.00 39.65 BBBB
ATOM   4932  CA  SER B 311      22.660 -32.714  -5.154  1.00 34.90 BBBB
ATOM   4938  CA  VAL B 312      21.990 -29.074  -4.341  1.00 31.50 BBBB
ATOM   4945  CA  ASP B 313      25.642 -28.202  -4.957  1.00 29.61 BBBB
ATOM   4953  CA  ALA B 314      25.782 -30.099  -8.254  1.00 26.47 BBBB
ATOM   4958  CA  VAL B 315      22.755 -28.215  -9.612  1.00 25.33 BBBB
ATOM   4965  CA  ALA B 316      23.888 -24.872  -8.199  1.00 27.13 BBBB
ATOM   4970  CA  ASN B 317      27.444 -25.246  -9.518  1.00 28.52 BBBB
ATOM   4978  CA  THR B 318      26.174 -26.371 -12.906  1.00 27.04 BBBB
ATOM   4985  CA  LEU B 319      23.883 -23.370 -13.357  1.00 25.21 BBBB
ATOM   4993  CA  ALA B 320      26.445 -20.931 -11.957  1.00 24.59 BBBB
ATOM   4998  CA  GLY B 321      28.934 -22.031 -14.591  1.00 24.34 BBBB
ATOM   5002  CA  TRP B 322      26.738 -21.007 -17.521  1.00 21.72 BBBB
ATOM   5016  CA  SER B 323      27.141 -17.404 -18.692  1.00 19.04 BBBB
ATOM   5022  CA  ARG B 324      24.725 -15.741 -21.112  1.00 18.09 BBBB
ATOM   5033  CA  GLU B 325      27.220 -16.368 -23.954  1.00 16.96 BBBB
ATOM   5042  CA  THR B 326      27.460 -20.055 -23.070  1.00 16.39 BBBB
ATOM   5049  CA  LEU B 327      23.659 -20.305 -22.780  1.00 17.27 BBBB
ATOM   5057  CA  LEU B 328      23.175 -18.745 -26.222  1.00 17.39 BBBB
ATOM   5065  CA  THR B 329      25.567 -21.335 -27.688  1.00 21.30 BBBB
ATOM   5072  CA  MET B 330      23.771 -24.153 -25.870  1.00 19.91 BBBB
ATOM   5080  CA  ALA B 331      20.412 -22.871 -27.098  1.00 18.49 BBBB
ATOM   5085  CA  GLU B 332      21.626 -22.827 -30.704  1.00 21.47 BBBB
ATOM   5094  CA  ARG B 333      23.040 -26.330 -30.408  1.00 23.77 BBBB
ATOM   5105  CA  ALA B 334      19.648 -27.420 -29.063  1.00 22.88 BBBB
ATOM   5110  CA  ARG B 335      17.795 -25.892 -32.002  1.00 23.54 BBBB
ATOM   5121  CA  ALA B 336      20.330 -27.477 -34.372  1.00 26.85 BBBB
ATOM   5126  CA  ALA B 337      19.740 -30.925 -32.865  1.00 30.89 BBBB
ATOM   5131  CA  SER B 338      16.008 -30.432 -33.408  1.00 32.41 BBBB
ATOM   5137  CA  ILE B 339      13.882 -31.941 -36.187  1.00 34.35 BBBB
ATOM   5146  CA  PRO B 340      10.733 -29.730 -36.600  1.00 34.94 BBBB
ATOM   5152  CA  ASP B 341       8.711 -31.820 -39.056  1.00 33.33 BBBB
ATOM   5160  CA  ALA B 342       8.875 -35.238 -37.411  1.00 29.09 BBBB
ATOM   5165  CA  THR B 343       5.115 -35.696 -37.744  1.00 28.55 BBBB
ATOM   5172  CA  GLU B 344       5.085 -34.933 -41.480  1.00 32.00 BBBB
ATOM   5181  CA  ARG B 345       8.138 -37.123 -42.067  1.00 31.44 BBBB
ATOM   5192  CA  VAL B 346       6.578 -40.151 -40.384  1.00 28.61 BBBB
ATOM   5199  CA  ALA B 347       3.249 -39.617 -42.137  1.00 28.96 BBBB
ATOM   5204  CA  ASN B 348       5.035 -39.286 -45.493  1.00 34.56 BBBB
ATOM   5212  CA  GLU B 349       6.954 -42.540 -44.956  1.00 34.86 BBBB
ATOM   5221  CA  VAL B 350       3.767 -44.306 -43.919  1.00 33.79 BBBB
ATOM   5228  CA  SER B 351       2.196 -42.946 -47.095  1.00 36.67 BBBB
ATOM   5234  CA  ARG B 352       5.114 -44.088 -49.251  1.00 40.03 BBBB
ATOM   5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78 BBBB
ATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24 BBBB
ATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71 BBBB
ATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93 BBBB
ATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81 BBBB
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END

TABLE 4 ATOMIC COORDINATES OF THE DONOR NUCLEOTIDE BINDING SITE

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REMARK    4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   LEU B 187      13.695 -22.128 -15.588  1.00 15.92      N
ATOM      2  CA  LEU B 187      12.361 -22.710 -15.604  1.00 16.75      C
ATOM      3  C   LEU B 187      12.450 -24.146 -15.085  1.00 16.85      C
ATOM      4  O   LEU B 187      13.115 -24.982 -15.688  1.00 17.18      O
ATOM      5  CB  LEU B 187      11.813 -22.701 -17.035  1.00 16.85      C
ATOM      6  CG  LEU B 187      10.445 -23.340 -17.276  1.00 18.63      C
ATOM      7  CD1 LEU B 187       9.368 -22.478 -16.625  1.00 19.42      C
ATOM      8  CD2 LEU B 187      10.198 -23.449 -18.783  1.00 19.11      C
ATOM      9  N   VAL B 188      11.788 -24.426 -13.964  1.00 18.20      N
ATOM     10  CA  VAL B 188      11.774 -25.775 -13.381  1.00 18.41      C
ATOM     11  C   VAL B 188      10.434 -26.440 -13.739  1.00 19.88      C
ATOM     12  O   VAL B 188       9.371 -25.967 -13.336  1.00 20.39      O
ATOM     13  CB  VAL B 188      11.902 -25.714 -11.842  1.00 18.98      C
ATOM     14  CG1 VAL B 188      12.088 -27.126 -11.270  1.00 18.50      C
ATOM     15  CG2 VAL B 188      13.061 -24.818 -11.449  1.00 18.83      C
ATOM     16  N   VAL B 189      10.493 -27.532 -14.496  1.00 21.55      N
ATOM     17  CA  VAL B 189       9.298 -28.234 -14.948  1.00 22.11      C
ATOM     18  C   VAL B 189       9.191 -29.639 -14.351  1.00 23.90      C
ATOM     19  O   VAL B 189      10.067 -30.478 -14.559  1.00 23.61      O
ATOM     20  CB  VAL B 189       9.299 -28.342 -16.488  1.00 22.50      C
ATOM     21  CG1 VAL B 189       8.009 -29.013 -16.981  1.00 22.70      C
ATOM     22  CG2 VAL B 189       9.470 -26.943 -17.101  1.00 21.26      C
ATOM     23  N   GLY B 190       8.111 -29.887 -13.615  1.00 25.60      N
ATOM     24  CA  GLY B 190       7.914 -31.188 -12.994  1.00 27.28      C
ATOM     25  C   GLY B 190       6.808 -32.026 -13.604  1.00 29.67      C
ATOM     26  O   GLY B 190       6.668 -33.208 -13.283  1.00 29.86      O
ATOM     27  N   GLY B 191       6.025 -31.430 -14.497  1.00 30.56      N
ATOM     28  CA  GLY B 191       4.935 -32.163 -15.115  1.00 31.94      C
ATOM     29  C   GLY B 191       3.676 -32.104 -14.269  1.00 33.11      C
ATOM     30  O   GLY B 191       3.691 -31.556 -13.165  1.00 32.14      O
ATOM     31  N   ALA B 195       7.761 -33.045  -9.938  1.00 33.54      N
ATOM     32  CA  ALA B 195       8.977 -33.819  -9.709  1.00 33.12      C
ATOM     33  C   ALA B 195       9.423 -33.590  -8.267  1.00 32.87      C
ATOM     34  O   ALA B 195       9.955 -32.533  -7.923  1.00 31.47      O
ATOM     35  CB  ALA B 195      10.073 -33.387 -10.679  1.00 33.17      C
ATOM     36  N   LEU B 198      12.897 -32.223  -7.590  1.00 27.07      N
ATOM     37  CA  LEU B 198      13.069 -30.833  -8.003  1.00 26.58      C
ATOM     38  C   LEU B 198      12.388 -29.893  -7.006  1.00 26.41      C
ATOM     39  O   LEU B 198      12.930 -28.835  -6.667  1.00 26.35      O
ATOM     40  CB  LEU B 198      12.504 -30.616  -9.412  1.00 25.88      C
ATOM     41  CG  LEU B 198      13.196 -31.408 -10.524  1.00 25.40      C
ATOM     42  CD1 LEU B 198      12.625 -31.007 -11.874  1.00 26.54      C
ATOM     43  CD2 LEU B 198      14.692 -31.146 -10.493  1.00 25.94      C
ATOM     44  N   TYR B 252       8.723 -21.314 -22.184  1.00 21.27      N
ATOM     45  CA  TYR B 252       9.972 -21.616 -22.886  1.00 22.78      C
ATOM     46  C   TYR B 252      10.566 -20.354 -23.516  1.00 23.57      C
ATOM     47  O   TYR B 252      11.784 -20.180 -23.550  1.00 23.91      O
ATOM     48  CB  TYR B 252       9.726 -22.661 -23.980  1.00 21.62      C
ATOM     49  CG  TYR B 252       9.662 -24.100 -23.505  1.00 23.34      C
ATOM     50  CD1 TYR B 252       9.003 -25.065 -24.261  1.00 22.88      C
ATOM     51  CD2 TYR B 252      10.288 -24.505 -22.319  1.00 22.30      C
ATOM     52  CE1 TYR B 252       8.961 -26.392 -23.861  1.00 24.81      C
ATOM     53  CE2 TYR B 252      10.253 -25.838 -21.912  1.00 23.56      C
ATOM     54  CZ  TYR B 252       9.590 -26.772 -22.687  1.00 24.26      C
ATOM     55  OH  TYR B 252       9.554 -28.088 -22.305  1.00 25.57      O
ATOM     56  N   VAL B 258      16.263 -24.643 -18.818  1.00 18.74      N
ATOM     57  CA  VAL B 258      15.208 -25.456 -18.234  1.00 19.32      C
ATOM     58  C   VAL B 258      15.799 -26.585 -17.389  1.00 19.70      C
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ATOM	59	O	VAL	B	258	16.808	-27.175	-17.758	1.00	18.96	O
ATOM	60	CB	VAL	B	258	14.328	-26.100	-19.337	1.00	19.89	C
ATOM	61	CG1	VAL	B	258	13.101	-26.754	-18.714	1.00	19.81	C
ATOM	62	CG2	VAL	B	258	13.907	-25.041	-20.364	1.00	21.59	C
ATOM	63	N	VAL	B	259	15.167	-26.861	-16.253	1.00	20.24	N
ATOM	64	CA	VAL	B	259	15.581	-27.957	-15.374	1.00	19.85	C
ATOM	65	C	VAL	B	259	14.382	-28.890	-15.371	1.00	20.02	C
ATOM	66	O	VAL	B	259	13.301	-28.500	-14.942	1.00	21.88	O
ATOM	67	CB	VAL	B	259	15.850	-27.483	-13.936	1.00	20.08	C
ATOM	68	CG1	VAL	B	259	16.222	-28.689	-13.059	1.00	20.22	C
ATOM	69	CG2	VAL	B	259	16.966	-26.453	-13.930	1.00	17.86	C
ATOM	70	N	CYS	B	260	14.562	-30.111	-15.867	1.00	21.70	N
ATOM	71	CA	CYS	B	260	13.454	-31.055	-15.946	1.00	22.00	C
ATOM	72	C	CYS	B	260	13.903	-32.478	-16.242	1.00	21.86	C
ATOM	73	O	CYS	B	260	15.087	-32.730	-16.496	1.00	21.34	O
ATOM	74	CB	CYS	B	260	12.494	-30.618	-17.057	1.00	22.77	C
ATOM	75	SG	CYS	B	260	13.297	-30.506	-18.711	1.00	22.15	S
ATOM	76	N	ARG	B	261	12.937	-33.397	-16.212	1.00	22.34	N
ATOM	77	CA	ARG	B	261	13.170	-34.800	-16.515	1.00	23.75	C
ATOM	78	C	ARG	B	261	13.351	-34.871	-18.032	1.00	23.98	C
ATOM	79	O	ARG	B	261	13.117	-33.883	-18.746	1.00	22.44	O
ATOM	80	CB	ARG	B	261	11.964	-35.663	-16.104	1.00	27.16	C
ATOM	81	CG	ARG	B	261	11.376	-35.337	-14.738	1.00	31.82	C
ATOM	82	CD	ARG	B	261	11.490	-36.473	-13.732	1.00	36.33	C
ATOM	83	NE	ARG	B	261	12.865	-36.721	-13.323	1.00	38.48	N
ATOM	84	CZ	ARG	B	261	13.218	-37.176	-12.125	1.00	37.25	C
ATOM	85	NH1	ARG	B	261	12.295	-37.433	-11.204	1.00	38.46	N
ATOM	86	NH2	ARG	B	261	14.499	-37.370	-11.848	1.00	36.79	N
ATOM	87	N	SER	B	262	13.740	-36.038	-18.527	1.00	22.00	N
ATOM	88	CA	SER	B	262	13.975	-36.189	-19.948	1.00	23.18	C
ATOM	89	C	SER	B	262	13.173	-37.263	-20.676	1.00	22.90	C
ATOM	90	O	SER	B	262	13.738	-38.179	-21.274	1.00	23.25	O
ATOM	91	CB	SER	B	262	15.481	-36.377	-20.203	1.00	24.45	C
ATOM	92	OG	SER	B	262	16.043	-37.326	-19.311	1.00	25.79	O
ATOM	93	N	GLY	B	263	11.850	-37.151	-20.619	1.00	22.74	N
ATOM	94	CA	GLY	B	263	11.026	-38.079	-21.361	1.00	22.85	C
ATOM	95	C	GLY	B	263	11.392	-37.793	-22.813	1.00	24.06	C
ATOM	96	O	GLY	B	263	11.908	-36.705	-23.121	1.00	22.75	O
ATOM	97	N	ALA	B	264	11.130	-38.739	-23.708	1.00	23.37	N
ATOM	98	CA	ALA	B	264	11.482	-38.564	-25.115	1.00	24.25	C
ATOM	99	C	ALA	B	264	10.843	-37.343	-25.783	1.00	24.29	C
ATOM	100	O	ALA	B	264	11.523	-36.572	-26.470	1.00	24.33	O
ATOM	101	CB	ALA	B	264	11.133	-39.829	-25.894	1.00	24.58	C
ATOM	102	N	LEU	B	265	9.541	-37.167	-25.596	1.00	24.44	N
ATOM	103	CA	LEU	B	265	8.846	-36.037	-26.205	1.00	24.66	C
ATOM	104	C	LEU	B	265	9.331	-34.717	-25.613	1.00	24.47	C
ATOM	105	O	LEU	B	265	9.374	-33.693	-26.301	1.00	23.85	O
ATOM	106	CB	LEU	B	265	7.332	-36.183	-26.011	1.00	25.33	C
ATOM	107	CG	LEU	B	265	6.760	-37.544	-26.426	1.00	27.97	C
ATOM	108	CD1	LEU	B	265	5.242	-37.541	-26.258	1.00	28.21	C
ATOM	109	CD2	LEU	B	265	7.146	-37.856	-27.878	1.00	27.40	C
ATOM	110	N	THR	B	266	9.702	-34.747	-24.338	1.00	22.12	N
ATOM	111	CA	THR	B	266	10.194	-33.557	-23.657	1.00	22.34	C
ATOM	112	C	THR	B	266	11.535	-33.117	-24.226	1.00	21.15	C
ATOM	113	O	THR	B	266	11.761	-31.926	-24.442	1.00	20.35	O
ATOM	114	CB	THR	B	266	10.348	-33.803	-22.140	1.00	22.35	C
ATOM	115	OG1	THR	B	266	9.061	-34.087	-21.583	1.00	24.46	O
ATOM	116	CG2	THR	B	266	10.945	-32.573	-21.444	1.00	24.00	C
ATOM	117	N	VAL	B	267	12.427	-34.075	-24.461	1.00	20.46	N
ATOM	118	CA	VAL	B	267	13.730	-33.762	-25.023	1.00	21.11	C
ATOM	119	C	VAL	B	267	13.548	-33.138	-26.416	1.00	21.34	C
ATOM	120	O	VAL	B	267	14.188	-32.135	-26.747	1.00	19.99	O
ATOM	121	CB	VAL	B	267	14.614	-35.039	-25.114	1.00	21.54	C
ATOM	122	CG1	VAL	B	267	15.903	-34.740	-25.865	1.00	20.72	C
ATOM	123	CG2	VAL	B	267	14.938	-35.541	-23.708	1.00	20.45	C
ATOM	124	N	SER	B	268	12.663	-33.717	-27.222	1.00	21.61	N

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ATOM    125  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96      C
ATOM    126  C   SER B 268      11.817 -31.790 -28.519  1.00 21.81      C
ATOM    127  O   SER B 268      12.158 -30.933 -29.336  1.00 22.60      O
ATOM    128  CB  SER B 268      11.474 -34.121 -29.344  1.00 21.57      C
ATOM    129  OG  SER B 268      12.141 -35.316 -29.721  1.00 24.06      O
ATOM    130  N   GLU B 269      10.928 -31.563 -27.557  1.00 21.64      N
ATOM    131  CA  GLU B 269      10.282 -30.272 -27.378  1.00 21.95      C
ATOM    132  C   GLU B 269      11.321 -29.214 -26.999  1.00 21.68      C
ATOM    133  O   GLU B 269      11.301 -28.095 -27.518  1.00 18.12      O
ATOM    134  CB  GLU B 269       9.213 -30.399 -26.292  1.00 24.72      C
ATOM    135  CG  GLU B 269       8.480 -29.128 -25.940  1.00 27.67      C
ATOM    136  CD  GLU B 269       7.385 -29.380 -24.908  1.00 30.05      C
ATOM    137  OE1 GLU B 269       6.325 -29.915 -25.287  1.00 31.50      O
ATOM    138  OE2 GLU B 269       7.591 -29.057 -23.719  1.00 29.84      O
ATOM    139  N   ILE B 270      12.224 -29.581 -26.092  1.00 19.43      N
ATOM    140  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62      C
ATOM    141  C   ILE B 270      14.214 -28.314 -26.806  1.00 20.58      C
ATOM    142  O   ILE B 270      14.595 -27.151 -26.954  1.00 20.50      O
ATOM    143  CB  ILE B 270      14.157 -29.391 -24.533  1.00 20.30      C
ATOM    144  CG1 ILE B 270      13.337 -29.574 -23.254  1.00 21.32      C
ATOM    145  CG2 ILE B 270      15.415 -28.595 -24.266  1.00 19.17      C
ATOM    146  CD1 ILE B 270      12.926 -28.291 -22.583  1.00 23.40      C
ATOM    147  N   ALA B 277      19.316 -27.110 -21.396  1.00 17.01      N
ATOM    148  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80      C
ATOM    149  C   ALA B 277      19.591 -28.526 -19.382  1.00 17.37      C
ATOM    150  O   ALA B 277      20.710 -28.891 -19.755  1.00 17.09      O
ATOM    151  CB  ALA B 277      17.641 -28.805 -20.895  1.00 17.01      C
ATOM    152  N   LEU B 278      19.147 -28.673 -18.138  1.00 17.14      N
ATOM    153  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48      C
ATOM    154  C   LEU B 278      18.884 -30.535 -16.898  1.00 19.62      C
ATOM    155  O   LEU B 278      17.870 -30.330 -16.218  1.00 20.77      O
ATOM    156  CB  LEU B 278      20.140 -28.619 -15.869  1.00 19.19      C
ATOM    157  CG  LEU B 278      21.084 -29.308 -14.868  1.00 20.85      C
ATOM    158  CD1 LEU B 278      21.283 -28.411 -13.668  1.00 21.11      C
ATOM    159  CD2 LEU B 278      20.497 -30.647 -14.433  1.00 19.16      C
ATOM    160  N   PHE B 279      19.149 -31.691 -17.495  1.00 19.50      N
ATOM    161  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59      C
ATOM    162  C   PHE B 279      18.525 -33.709 -16.167  1.00 22.86      C
ATOM    163  O   PHE B 279      19.671 -34.065 -15.871  1.00 23.32      O
ATOM    164  CB  PHE B 279      18.385 -33.700 -18.651  1.00 21.07      C
ATOM    165  CG  PHE B 279      17.740 -33.099 -19.876  1.00 19.35      C
ATOM    166  CD1 PHE B 279      18.481 -32.898 -21.035  1.00 19.42      C
ATOM    167  CD2 PHE B 279      16.379 -32.794 -19.888  1.00 18.16      C
ATOM    168  CE1 PHE B 279      17.874 -32.405 -22.203  1.00 19.06      C
ATOM    169  CE2 PHE B 279      15.759 -32.298 -21.052  1.00 17.65      C
ATOM    170  CZ  PHE B 279      16.515 -32.108 -22.208  1.00 15.61      C
ATOM    171  N   VAL B 280      17.445 -34.037 -15.461  1.00 23.88      N
ATOM    172  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67      C
ATOM    173  C   VAL B 280      16.690 -36.136 -14.658  1.00 25.65      C
ATOM    174  O   VAL B 280      15.509 -36.239 -14.346  1.00 24.57      O
ATOM    175  CB  VAL B 280      16.883 -34.223 -13.048  1.00 26.89      C
ATOM    176  CG1 VAL B 280      16.954 -35.159 -11.847  1.00 28.12      C
ATOM    177  CG2 VAL B 280      17.631 -32.929 -12.742  1.00 27.70      C
ATOM    178  N   PRO B 281      17.324 -37.080 -15.370  1.00 27.08      N
ATOM    179  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05      C
ATOM    180  C   PRO B 281      16.092 -39.121 -14.684  1.00 31.51      C
ATOM    181  O   PRO B 281      16.675 -39.223 -13.603  1.00 32.26      O
ATOM    182  CB  PRO B 281      17.851 -39.071 -16.492  1.00 29.44      C
ATOM    183  CG  PRO B 281      18.791 -37.992 -16.895  1.00 29.67      C
ATOM    184  CD  PRO B 281      18.750 -37.057 -15.726  1.00 27.31      C
ATOM    185  N   PHE B 282      14.908 -39.668 -14.923  1.00 33.83      N
ATOM    186  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13      C
ATOM    187  C   PHE B 282      15.078 -41.776 -13.880  1.00 38.09      C
ATOM    188  O   PHE B 282      15.357 -42.373 -14.921  1.00 38.33      O
ATOM    189  CB  PHE B 282      12.818 -40.808 -14.372  1.00 38.38      C
ATOM    190  CG  PHE B 282      12.032 -41.606 -13.377  1.00 40.57      C
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ATOM	191	CD1	PHE	B	282	11.720	-41.074	-12.130	1.00	41.80	C
ATOM	192	CD2	PHE	B	282	11.590	-42.886	-13.689	1.00	41.65	C
ATOM	193	CE1	PHE	B	282	10.975	-41.806	-11.209	1.00	42.03	C
ATOM	194	CE2	PHE	B	282	10.843	-43.628	-12.773	1.00	42.49	C
ATOM	195	CZ	PHE	B	282	10.536	-43.085	-11.532	1.00	41.74	C
ATOM	196	N	GLN	B	288	16.212	-45.321	-19.533	1.00	30.94	N
ATOM	197	CA	GLN	B	288	15.622	-44.804	-20.755	1.00	30.77	C
ATOM	198	C	GLN	B	288	15.783	-43.291	-20.885	1.00	29.70	C
ATOM	199	O	GLN	B	288	16.268	-42.801	-21.902	1.00	29.79	O
ATOM	200	CB	GLN	B	288	14.143	-45.158	-20.810	1.00	30.59	C
ATOM	201	CG	GLN	B	288	13.473	-44.772	-22.109	1.00	29.73	C
ATOM	202	CD	GLN	B	288	11.981	-44.971	-22.044	1.00	28.04	C
ATOM	203	OE1	GLN	B	288	11.294	-44.295	-21.279	1.00	29.59	O
ATOM	204	NE2	GLN	B	288	11.468	-45.905	-22.838	1.00	26.98	N
ATOM	205	N	GLN	B	289	15.378	-42.554	-19.857	1.00	29.38	N
ATOM	206	CA	GLN	B	289	15.474	-41.099	-19.904	1.00	29.46	C
ATOM	207	C	GLN	B	289	16.906	-40.613	-20.005	1.00	29.36	C
ATOM	208	O	GLN	B	289	17.173	-39.557	-20.585	1.00	29.12	O
ATOM	209	CB	GLN	B	289	14.772	-40.472	-18.700	1.00	29.25	C
ATOM	210	CG	GLN	B	289	13.265	-40.416	-18.883	1.00	29.32	C
ATOM	211	CD	GLN	B	289	12.575	-39.585	-17.826	1.00	29.84	C
ATOM	212	OE1	GLN	B	289	13.191	-38.728	-17.188	1.00	29.52	O
ATOM	213	NE2	GLN	B	289	11.281	-39.821	-17.647	1.00	28.95	N
ATOM	214	N	TYR	B	290	17.835	-41.374	-19.442	1.00	28.95	N
ATOM	215	CA	TYR	B	290	19.228	-40.984	-19.550	1.00	29.55	C
ATOM	216	C	TYR	B	290	19.593	-41.042	-21.032	1.00	28.80	C
ATOM	217	O	TYR	B	290	20.192	-40.113	-21.567	1.00	29.22	O
ATOM	218	CB	TYR	B	290	20.136	-41.934	-18.768	1.00	31.40	C
ATOM	219	CG	TYR	B	290	21.587	-41.780	-19.148	1.00	33.37	C
ATOM	220	CD1	TYR	B	290	22.332	-40.682	-18.717	1.00	34.57	C
ATOM	221	CD2	TYR	B	290	22.192	-42.684	-20.017	1.00	34.90	C
ATOM	222	CE1	TYR	B	290	23.644	-40.490	-19.148	1.00	35.97	C
ATOM	223	CE2	TYR	B	290	23.497	-42.500	-20.453	1.00	36.03	C
ATOM	224	CZ	TYR	B	290	24.214	-41.402	-20.019	1.00	36.29	C
ATOM	225	OH	TYR	B	290	25.499	-41.215	-20.475	1.00	39.44	O
ATOM	226	N	ASN	B	292	17.658	-40.779	-23.508	1.00	25.52	N
ATOM	227	CA	ASN	B	292	16.902	-39.784	-24.270	1.00	26.06	C
ATOM	228	C	ASN	B	292	17.605	-38.427	-24.258	1.00	25.99	C
ATOM	229	O	ASN	B	292	17.566	-37.687	-25.244	1.00	26.18	O
ATOM	230	CB	ASN	B	292	15.484	-39.599	-23.709	1.00	24.78	C
ATOM	231	CG	ASN	B	292	14.590	-40.811	-23.928	1.00	24.46	C
ATOM	232	OD1	ASN	B	292	14.842	-41.641	-24.798	1.00	25.33	O
ATOM	233	ND2	ASN	B	292	13.523	-40.900	-23.146	1.00	23.83	N
ATOM	234	N	ALA	B	293	18.242	-38.105	-23.139	1.00	25.66	N
ATOM	235	CA	ALA	B	293	18.926	-36.822	-22.979	1.00	25.69	C
ATOM	236	C	ALA	B	293	20.346	-36.800	-23.521	1.00	25.67	C
ATOM	237	O	ALA	B	293	20.855	-35.743	-23.902	1.00	25.52	O
ATOM	238	CB	ALA	B	293	18.940	-36.422	-21.506	1.00	24.17	C
ATOM	239	N	LEU	B	296	21.375	-34.703	-26.688	1.00	25.66	N
ATOM	240	CA	LEU	B	296	21.521	-33.265	-26.481	1.00	25.42	C
ATOM	241	C	LEU	B	296	22.784	-32.935	-25.688	1.00	26.07	C
ATOM	242	O	LEU	B	296	23.435	-31.917	-25.944	1.00	25.26	O
ATOM	243	CB	LEU	B	296	20.283	-32.685	-25.779	1.00	24.45	C
ATOM	244	CG	LEU	B	296	19.066	-32.458	-26.679	1.00	25.59	C
ATOM	245	CD1	LEU	B	296	17.968	-31.718	-25.911	1.00	23.56	C
ATOM	246	CD2	LEU	B	296	19.496	-31.630	-27.893	1.00	25.87	C
ATOM	247	N	ALA	B	302	23.066	-29.504	-23.507	1.00	20.94	N
ATOM	248	CA	ALA	B	302	22.516	-29.770	-22.186	1.00	21.78	C
ATOM	249	C	ALA	B	302	23.503	-30.507	-21.288	1.00	22.69	C
ATOM	250	O	ALA	B	302	24.561	-30.948	-21.739	1.00	22.25	O
ATOM	251	CB	ALA	B	302	21.243	-30.595	-22.327	1.00	20.10	C
ATOM	252	N	LYS	B	303	23.156	-30.613	-20.009	1.00	24.62	N
ATOM	253	CA	LYS	B	303	23.979	-31.340	-19.048	1.00	25.86	C
ATOM	254	C	LYS	B	303	23.083	-32.319	-18.302	1.00	26.41	C
ATOM	255	O	LYS	B	303	22.015	-31.948	-17.802	1.00	25.76	O
ATOM	256	CB	LYS	B	303	24.632	-30.401	-18.036	1.00	27.65	C

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ATOM    257  CG  LYS B 303      25.466 -31.146 -16.986  1.00 29.37      C
ATOM    258  CD  LYS B 303      26.150 -30.186 -16.025  1.00 32.41      C
ATOM    259  CE  LYS B 303      27.083 -30.912 -15.056  1.00 33.22      C
ATOM    260  NZ  LYS B 303      27.827 -29.952 -14.181  1.00 33.62      N
ATOM    261  N   ILE B 304      23.520 -33.570 -18.234  1.00 25.65      N
ATOM    262  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17      C
ATOM    263  C   ILE B 304      23.308 -34.855 -16.160  1.00 27.00      C
ATOM    264  O   ILE B 304      24.511 -35.012 -15.986  1.00 27.46      O
ATOM    265  CB  ILE B 304      22.786 -35.946 -18.316  1.00 27.06      C
ATOM    266  CG1 ILE B 304      22.242 -35.769 -19.733  1.00 27.61      C
ATOM    267  CG2 ILE B 304      21.977 -36.996 -17.555  1.00 28.49      C
ATOM    268  CD1 ILE B 304      22.380 -37.009 -20.599  1.00 27.05      C
ATOM    269  N   ILE B 305      22.428 -34.869 -15.168  1.00 27.22      N
ATOM    270  CA  ILE B 305      22.843 -35.178 -13.813  1.00 29.01      C
ATOM    271  C   ILE B 305      21.934 -36.302 -13.351  1.00 29.64      C
ATOM    272  O   ILE B 305      20.806 -36.067 -12.932  1.00 29.25      O
ATOM    273  CB  ILE B 305      22.713 -33.977 -12.858  1.00 28.91      C
ATOM    274  CG1 ILE B 305      23.660 -32.855 -13.299  1.00 29.51      C
ATOM    275  CG2 ILE B 305      23.063 -34.416 -11.432  1.00 30.98      C
ATOM    276  CD1 ILE B 305      23.674 -31.653 -12.367  1.00 29.43      C
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TABLE 5 ATOMIC COORDINATES OF ACCEPTOR BINDING SITE

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REMARK    4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   MET B  12      -0.734 -48.902 -33.817  1.00 23.68      N
ATOM      2  CA  MET B  12      -0.523 -49.707 -32.613  1.00 24.54      C
ATOM      3  C   MET B  12       0.361 -48.840 -31.720  1.00 25.31      C
ATOM      4  O   MET B  12       1.546 -48.645 -32.006  1.00 23.88      O
ATOM      5  CB  MET B  12       0.192 -51.019 -32.971  1.00 24.28      C
ATOM      6  CG  MET B  12      -0.402 -51.726 -34.188  1.00 25.19      C
ATOM      7  SD  MET B  12       0.399 -53.284 -34.669  1.00 26.54      S
ATOM      8  CE  MET B  12       1.990 -52.691 -35.289  1.00 22.99      C
ATOM      9  N   ALA B  13      -0.224 -48.292 -30.657  1.00 27.08      N
ATOM     10  CA  ALA B  13       0.508 -47.410 -29.752  1.00 29.43      C
ATOM     11  C   ALA B  13      -0.239 -47.192 -28.436  1.00 31.80      C
ATOM     12  O   ALA B  13      -1.143 -46.350 -28.352  1.00 32.16      O
ATOM     13  CB  ALA B  13       0.747 -46.074 -30.429  1.00 28.82      C
ATOM     14  N   GLY B  14       0.150 -47.934 -27.405  1.00 32.46      N
ATOM     15  CA  GLY B  14      -0.513 -47.804 -26.120  1.00 33.82      C
ATOM     16  C   GLY B  14      -0.107 -46.595 -25.299  1.00 34.82      C
ATOM     17  O   GLY B  14       0.975 -46.040 -25.479  1.00 35.47      O
ATOM     18  N   GLY B  15      -0.986 -46.188 -24.385  1.00 35.56      N
ATOM     19  CA  GLY B  15      -0.700 -45.047 -23.536  1.00 36.08      C
ATOM     20  C   GLY B  15       0.539 -45.254 -22.683  1.00 36.84      C
ATOM     21  O   GLY B  15       1.293 -44.311 -22.426  1.00 36.03      O
ATOM     22  N   THR B  16       0.755 -46.488 -22.240  1.00 36.65      N
ATOM     23  CA  THR B  16       1.920 -46.787 -21.421  1.00 38.51      C
ATOM     24  C   THR B  16       3.158 -46.497 -22.264  1.00 38.35      C
ATOM     25  O   THR B  16       3.191 -46.798 -23.460  1.00 39.90      O
ATOM     26  CB  THR B  16       1.926 -48.258 -20.974  1.00 38.51      C
ATOM     27  OG1 THR B  16       0.686 -48.558 -20.321  1.00 38.39      O
ATOM     28  CG2 THR B  16       3.075 -48.518 -20.005  1.00 39.11      C
ATOM     29  N   GLY B  17       4.168 -45.897 -21.649  1.00 37.68      N
ATOM     30  CA  GLY B  17       5.367 -45.567 -22.392  1.00 36.57      C
ATOM     31  C   GLY B  17       5.161 -44.303 -23.211  1.00 35.56      C
ATOM     32  O   GLY B  17       6.079 -43.843 -23.890  1.00 35.03      O
ATOM     33  N   GLY B  18       3.949 -43.752 -23.150  1.00 33.83      N
ATOM     34  CA  GLY B  18       3.631 -42.529 -23.872  1.00 33.48      C
ATOM     35  C   GLY B  18       3.825 -42.593 -25.378  1.00 33.12      C
ATOM     36  O   GLY B  18       4.345 -41.650 -25.984  1.00 35.38      O
ATOM     37  N   HIS B  19       3.416 -43.699 -25.988  1.00 30.26      N
ATOM     38  CA  HIS B  19       3.548 -43.865 -27.435  1.00 28.22      C
ATOM     39  C   HIS B  19       2.280 -43.370 -28.144  1.00 27.91      C
ATOM     40  O   HIS B  19       2.300 -43.049 -29.337  1.00 26.91      O
ATOM     41  CB  HIS B  19       3.772 -45.349 -27.779  1.00 25.81      C
ATOM     42  CG  HIS B  19       4.957 -45.966 -27.094  1.00 25.35      C
ATOM     43  ND1 HIS B  19       4.845 -47.025 -26.217  1.00 24.57      N
ATOM     44  CD2 HIS B  19       6.281 -45.694 -27.184  1.00 24.18      C
ATOM     45  CE1 HIS B  19       6.046 -47.380 -25.798  1.00 23.08      C
ATOM     46  NE2 HIS B  19       6.936 -46.589 -26.369  1.00 25.51      N
ATOM     47  N   VAL B  20       1.180 -43.310 -27.402  1.00 27.65      N
ATOM     48  CA  VAL B  20      -0.098 -42.894 -27.965  1.00 27.77      C
ATOM     49  C   VAL B  20      -0.140 -41.452 -28.470  1.00 27.57      C
ATOM     50  O   VAL B  20      -0.771 -41.172 -29.486  1.00 27.12      O
ATOM     51  CB  VAL B  20      -1.248 -43.080 -26.942  1.00 28.57      C
ATOM     52  CG1 VAL B  20      -1.082 -42.114 -25.787  1.00 30.03      C
ATOM     53  CG2 VAL B  20      -2.602 -42.873 -27.631  1.00 26.82      C
ATOM     54  N   LEU B  40      -5.323 -50.004 -32.549  1.00 25.21      N
ATOM     55  CA  LEU B  40      -5.200 -51.364 -32.026  1.00 24.71      C
ATOM     56  C   LEU B  40      -4.535 -51.235 -30.655  1.00 23.33      C
ATOM     57  O   LEU B  40      -3.387 -50.824 -30.563  1.00 23.43      O
ATOM     58  CB  LEU B  40      -4.326 -52.221 -32.952  1.00 25.21      C
ATOM     59  CG  LEU B  40      -4.416 -53.754 -32.868  1.00 26.95      C
ATOM     60  CD1 LEU B  40      -3.037 -54.334 -32.571  1.00 27.63      C
ATOM     61  CD2 LEU B  40      -5.421 -54.179 -31.817  1.00 26.69      C
ATOM     62  N   GLU B  47      -4.976 -45.941 -23.678  1.00 32.85      N
ATOM     63  CA  GLU B  47      -5.458 -45.655 -25.029  1.00 31.79      C
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ATOM     64  C   GLU B  47      -6.938 -46.017 -25.191  1.00 31.81      C
ATOM     65  O   GLU B  47      -7.626 -45.476 -26.055  1.00 31.31      O
ATOM     66  CB  GLU B  47      -4.624 -46.402 -26.080  1.00 30.62      C
ATOM     67  CG  GLU B  47      -4.755 -47.922 -26.051  1.00 29.85      C
ATOM     68  CD  GLU B  47      -3.793 -48.597 -25.082  1.00 29.78      C
ATOM     69  OE1 GLU B  47      -3.188 -47.895 -24.247  1.00 28.76      O
ATOM     70  OE2 GLU B  47      -3.649 -49.840 -25.156  1.00 29.01      O
ATOM     71  N   ILE B  63      -3.428 -59.342 -24.313  1.00 30.07      N
ATOM     72  CA  ILE B  63      -2.036 -59.770 -24.231  1.00 31.38      C
ATOM     73  C   ILE B  63      -1.623 -59.981 -22.775  1.00 33.08      C
ATOM     74  O   ILE B  63      -0.444 -59.872 -22.430  1.00 33.21      O
ATOM     75  CB  ILE B  63      -1.081 -58.745 -24.883  1.00 30.06      C
ATOM     76  CG1 ILE B  63      -1.143 -57.411 -24.137  1.00 29.94      C
ATOM     77  CG2 ILE B  63      -1.442 -58.567 -26.353  1.00 30.41      C
ATOM     78  CD1 ILE B  63      -0.128 -56.384 -24.632  1.00 29.62      C
ATOM     79  N   ARG B  67       2.953 -59.185 -21.440  1.00 31.54      N
ATOM     80  CA  ARG B  67       3.671 -57.928 -21.277  1.00 30.90      C
ATOM     81  C   ARG B  67       5.071 -58.142 -20.713  1.00 29.99      C
ATOM     82  O   ARG B  67       5.294 -59.034 -19.889  1.00 28.67      O
ATOM     83  CB  ARG B  67       2.888 -56.984 -20.363  1.00 32.28      C
ATOM     84  CG  ARG B  67       1.540 -56.576 -20.913  1.00 34.65      C
ATOM     85  CD  ARG B  67       0.926 -55.440 -20.097  1.00 36.69      C
ATOM     86  NE  ARG B  67      -0.259 -54.889 -20.748  1.00 38.28      N
ATOM     87  CZ  ARG B  67      -1.425 -55.519 -20.853  1.00 39.05      C
ATOM     88  NH1 ARG B  67      -1.583 -56.734 -20.341  1.00 39.61      N
ATOM     89  NH2 ARG B  67      -2.434 -54.935 -21.487  1.00 39.52      N
ATOM     90  N   GLY B  68       6.014 -57.321 -21.165  1.00 27.75      N
ATOM     91  CA  GLY B  68       7.380 -57.427 -20.685  1.00 26.79      C
ATOM     92  C   GLY B  68       8.166 -58.579 -21.280  1.00 25.41      C
ATOM     93  O   GLY B  68       9.326 -58.779 -20.943  1.00 26.04      O
ATOM     94  N   GLY B 102       3.556 -48.986 -35.936  1.00 20.96      N
ATOM     95  CA  GLY B 102       3.796 -49.357 -34.549  1.00 19.23      C
ATOM     96  C   GLY B 102       4.655 -48.282 -33.918  1.00 18.45      C
ATOM     97  O   GLY B 102       5.765 -48.016 -34.381  1.00 18.70      O
ATOM     98  N   MET B 103       4.155 -47.660 -32.857  1.00 18.01      N
ATOM     99  CA  MET B 103       4.892 -46.597 -32.191  1.00 18.93      C
ATOM    100  C   MET B 103       5.612 -47.128 -30.957  1.00 18.98      C
ATOM    101  O   MET B 103       6.134 -46.357 -30.158  1.00 17.96      O
ATOM    102  CB  MET B 103       3.928 -45.477 -31.781  1.00 20.02      C
ATOM    103  CG  MET B 103       3.121 -44.888 -32.944  1.00 21.61      C
ATOM    104  SD  MET B 103       4.212 -44.135 -34.157  1.00 23.45      S
ATOM    105  CE  MET B 103       4.718 -42.680 -33.271  1.00 21.40      C
ATOM    106  N   GLY B 104       5.640 -48.450 -30.827  1.00 21.56      N
ATOM    107  CA  GLY B 104       6.275 -49.080 -29.686  1.00 21.89      C
ATOM    108  C   GLY B 104       5.192 -49.614 -28.764  1.00 23.28      C
ATOM    109  O   GLY B 104       4.009 -49.353 -28.980  1.00 22.50      O
ATOM    110  N   GLY B 105       5.583 -50.364 -27.741  1.00 23.01      N
ATOM    111  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54      C
ATOM    112  C   GLY B 105       4.358 -52.380 -27.078  1.00 23.17      C
ATOM    113  O   GLY B 105       4.449 -52.844 -28.214  1.00 22.69      O
ATOM    114  N   TYR B 106       4.018 -53.118 -26.026  1.00 22.87      N
ATOM    115  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37      C
ATOM    116  C   TYR B 106       2.719 -55.018 -27.100  1.00 20.52      C
ATOM    117  O   TYR B 106       2.867 -56.052 -27.746  1.00 20.50      O
ATOM    118  CB  TYR B 106       3.632 -55.181 -24.774  1.00 25.08      C
ATOM    119  CG  TYR B 106       4.864 -55.008 -23.929  1.00 28.19      C
ATOM    120  CD1 TYR B 106       4.869 -54.153 -22.830  1.00 31.96      C
ATOM    121  CD2 TYR B 106       6.058 -55.631 -24.282  1.00 31.27      C
ATOM    122  CE1 TYR B 106       6.043 -53.915 -22.108  1.00 33.13      C
ATOM    123  CE2 TYR B 106       7.234 -55.400 -23.569  1.00 32.27      C
ATOM    124  CZ  TYR B 106       7.219 -54.541 -22.487  1.00 33.19      C
ATOM    125  OH  TYR B 106       8.388 -54.291 -21.802  1.00 35.95      O
ATOM    126  N   VAL B 107       1.628 -54.270 -27.205  1.00 19.06      N
ATOM    127  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06      C
ATOM    128  C   VAL B 107       1.015 -54.743 -29.559  1.00 17.45      C
ATOM    129  O   VAL B 107       0.502 -55.536 -30.346  1.00 16.99      O
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ATOM	130	CB	VAL	B	107	-0.690	-53.774	-27.978	1.00 20.95	C
ATOM	131	CG1	VAL	B	107	-0.407	-52.407	-28.589	1.00 21.39	C
ATOM	132	CG2	VAL	B	107	-1.879	-54.433	-28.658	1.00 21.30	C
ATOM	133	N	SER	B	108	1.991	-53.916	-29.918	1.00 17.96	N
ATOM	134	CA	SER	B	108	2.488	-53.892	-31.290	1.00 19.67	C
ATOM	135	C	SER	B	108	3.197	-55.187	-31.694	1.00 20.38	C
ATOM	136	O	SER	B	108	3.385	-55.449	-32.884	1.00 21.25	O
ATOM	137	CB	SER	B	108	3.424	-52.691	-31.508	1.00 19.56	C
ATOM	138	OG	SER	B	108	4.666	-52.824	-30.837	1.00 19.63	O
ATOM	139	N	GLY	B	109	3.595	-55.995	-30.710	1.00 19.59	N
ATOM	140	CA	GLY	B	109	4.251	-57.256	-31.023	1.00 20.03	C
ATOM	141	C	GLY	B	109	3.311	-58.170	-31.792	1.00 19.61	C
ATOM	142	O	GLY	B	109	3.579	-58.517	-32.940	1.00 19.24	O
ATOM	143	N	PRO	B	110	2.206	-58.606	-31.173	1.00 19.20	N
ATOM	144	CA	PRO	B	110	1.251	-59.478	-31.855	1.00 18.99	C
ATOM	145	C	PRO	B	110	0.651	-58.761	-33.075	1.00 19.22	C
ATOM	146	O	PRO	B	110	0.406	-59.371	-34.116	1.00 17.13	O
ATOM	147	CB	PRO	B	110	0.198	-59.737	-30.778	1.00 20.41	C
ATOM	148	CG	PRO	B	110	0.998	-59.720	-29.515	1.00 19.81	C
ATOM	149	CD	PRO	B	110	1.914	-58.528	-29.729	1.00 19.94	C
ATOM	150	N	HIS	B	125	8.182	-46.638	-35.447	1.00 21.40	N
ATOM	151	CA	HIS	B	125	8.814	-45.413	-34.981	1.00 21.42	C
ATOM	152	C	HIS	B	125	9.196	-45.642	-33.519	1.00 21.70	C
ATOM	153	O	HIS	B	125	8.378	-46.117	-32.725	1.00 19.81	O
ATOM	154	CB	HIS	B	125	7.858	-44.218	-35.067	1.00 21.57	C
ATOM	155	CG	HIS	B	125	8.432	-42.948	-34.511	1.00 23.73	C
ATOM	156	ND1	HIS	B	125	9.274	-42.127	-35.236	1.00 26.23	N
ATOM	157	CD2	HIS	B	125	8.300	-42.368	-33.295	1.00 22.15	C
ATOM	158	CE1	HIS	B	125	9.631	-41.095	-34.490	1.00 24.20	C
ATOM	159	NE2	HIS	B	125	9.054	-41.218	-33.307	1.00 26.07	N
ATOM	160	N	GLU	B	126	10.444	-45.332	-33.186	1.00 21.20	N
ATOM	161	CA	GLU	B	126	10.947	-45.452	-31.817	1.00 22.15	C
ATOM	162	C	GLU	B	126	11.205	-44.027	-31.326	1.00 21.93	C
ATOM	163	O	GLU	B	126	12.016	-43.300	-31.908	1.00 21.33	O
ATOM	164	CB	GLU	B	126	12.252	-46.246	-31.790	1.00 21.99	C
ATOM	165	CG	GLU	B	126	12.958	-46.206	-30.439	1.00 22.04	C
ATOM	166	CD	GLU	B	126	12.119	-46.824	-29.338	1.00 21.43	C
ATOM	167	OE1	GLU	B	126	11.767	-48.014	-29.471	1.00 21.92	O
ATOM	168	OE2	GLU	B	126	11.807	-46.124	-28.349	1.00 21.08	O
ATOM	169	N	GLN	B	127	10.520	-43.624	-30.259	1.00 22.62	N
ATOM	170	CA	GLN	B	127	10.682	-42.270	-29.735	1.00 22.81	C
ATOM	171	C	GLN	B	127	11.874	-42.087	-28.809	1.00 22.39	C
ATOM	172	O	GLN	B	127	12.399	-40.976	-28.682	1.00 22.43	O
ATOM	173	CB	GLN	B	127	9.414	-41.814	-28.989	1.00 23.56	C
ATOM	174	CG	GLN	B	127	8.147	-41.783	-29.830	1.00 24.46	C
ATOM	175	CD	GLN	B	127	7.312	-43.041	-29.687	1.00 25.85	C
ATOM	176	OE1	GLN	B	127	6.842	-43.366	-28.591	1.00 23.78	O
ATOM	177	NE2	GLN	B	127	7.119	-43.758	-30.797	1.00 24.91	N
ATOM	178	N	ASN	B	128	12.314	-43.173	-28.177	1.00 22.35	N
ATOM	179	CA	ASN	B	128	13.406	-43.097	-27.216	1.00 22.96	C
ATOM	180	C	ASN	B	128	14.824	-43.314	-27.742	1.00 23.87	C
ATOM	181	O	ASN	B	128	15.026	-43.856	-28.830	1.00 24.05	O
ATOM	182	CB	ASN	B	128	13.136	-44.080	-26.064	1.00 22.85	C
ATOM	183	CG	ASN	B	128	11.742	-43.919	-25.474	1.00 23.25	C
ATOM	184	OD1	ASN	B	128	10.804	-44.632	-25.848	1.00 26.04	O
ATOM	185	ND2	ASN	B	128	11.597	-42.975	-24.556	1.00 22.68	N
ATOM	186	N	GLY	B	132	12.851	-49.814	-27.506	1.00 24.52	N
ATOM	187	CA	GLY	B	132	12.007	-50.532	-26.568	1.00 24.05	C
ATOM	188	C	GLY	B	132	12.150	-52.019	-26.831	1.00 23.35	C
ATOM	189	O	GLY	B	132	12.582	-52.419	-27.904	1.00 22.89	O
ATOM	190	N	LEU	B	133	11.788	-52.846	-25.860	1.00 23.38	N
ATOM	191	CA	LEU	B	133	11.903	-54.293	-26.020	1.00 24.54	C
ATOM	192	C	LEU	B	133	11.209	-54.833	-27.276	1.00 22.84	C
ATOM	193	O	LEU	B	133	11.784	-55.619	-28.027	1.00 21.86	O
ATOM	194	CB	LEU	B	133	11.328	-54.996	-24.786	1.00 25.48	C
ATOM	195	CG	LEU	B	133	11.388	-56.527	-24.780	1.00 27.50	C

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ATOM    196  CD1 LEU B 133      12.840 -56.984 -24.866  1.00 28.69      C
ATOM    197  CD2 LEU B 133      10.735 -57.059 -23.509  1.00 28.04      C
ATOM    198  N   THR B 134       9.975 -54.401 -27.499  1.00 21.72      N
ATOM    199  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22      C
ATOM    200  C   THR B 134       9.693 -54.326 -29.986  1.00 20.62      C
ATOM    201  O   THR B 134       9.843 -55.091 -30.932  1.00 20.33      O
ATOM    202  CB  THR B 134       7.716 -54.509 -28.449  1.00 20.99      C
ATOM    203  OG1 THR B 134       7.257 -55.075 -27.210  1.00 20.94      O
ATOM    204  CG2 THR B 134       6.872 -55.073 -29.600  1.00 20.64      C
ATOM    205  N   ASN B 135       9.932 -53.021 -30.075  1.00 21.24      N
ATOM    206  CA  ASN B 135      10.407 -52.419 -31.324  1.00 20.50      C
ATOM    207  C   ASN B 135      11.724 -53.064 -31.767  1.00 20.78      C
ATOM    208  O   ASN B 135      11.945 -53.290 -32.953  1.00 20.41      O
ATOM    209  CB  ASN B 135      10.637 -50.911 -31.142  1.00 19.58      C
ATOM    210  CG  ASN B 135       9.457 -50.058 -31.597  1.00 19.93      C
ATOM    211  OD1 ASN B 135       9.454 -48.837 -31.390  1.00 21.78      O
ATOM    212  ND2 ASN B 135       8.467 -50.677 -32.219  1.00 17.21      N
ATOM    213  N   LEU B 138      10.741 -56.381 -33.386  1.00 21.61      N
ATOM    214  CA  LEU B 138       9.744 -56.188 -34.431  1.00 23.15      C
ATOM    215  C   LEU B 138      10.384 -55.558 -35.676  1.00 23.07      C
ATOM    216  O   LEU B 138       9.958 -55.801 -36.809  1.00 22.68      O
ATOM    217  CB  LEU B 138       8.618 -55.305 -33.886  1.00 23.87      C
ATOM    218  CG  LEU B 138       7.312 -55.155 -34.664  1.00 26.48      C
ATOM    219  CD1 LEU B 138       6.672 -56.508 -34.915  1.00 25.34      C
ATOM    220  CD2 LEU B 138       6.383 -54.267 -33.851  1.00 25.90      C
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TABLE 6 ATOMIC COORDINATES OF MEMBRANE ASSOCIATION SITE

REMARK	4	1MUR	COMPLIES	WITH	FORMAT	V.	2.0,	11-MAY-2000		
ATOM	1	N	MET	B	12	-0.734	-48.902	-33.817	1.00	23.68	N
ATOM	2	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	C
ATOM	3	C	MET	B	12	0.361	-48.840	-31.720	1.00	25.31	C
ATOM	4	O	MET	B	12	1.546	-48.645	-32.006	1.00	23.88	O
ATOM	5	CB	MET	B	12	0.192	-51.019	-32.971	1.00	24.28	C
ATOM	6	CG	MET	B	12	-0.402	-51.726	-34.188	1.00	25.19	C
ATOM	7	SD	MET	B	12	0.399	-53.284	-34.669	1.00	26.54	S
ATOM	8	CE	MET	B	12	1.990	-52.691	-35.289	1.00	22.99	C
ATOM	9	N	LEU	B	40	-5.323	-50.004	-32.549	1.00	25.21	N
ATOM	10	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71	C
ATOM	11	C	LEU	B	40	-4.535	-51.235	-30.655	1.00	23.33	C
ATOM	12	O	LEU	B	40	-3.387	-50.824	-30.563	1.00	23.43	O
ATOM	13	CB	LEU	B	40	-4.326	-52.221	-32.952	1.00	25.21	C
ATOM	14	CG	LEU	B	40	-4.416	-53.754	-32.868	1.00	26.95	C
ATOM	15	CD1	LEU	B	40	-3.037	-54.334	-32.571	1.00	27.63	C
ATOM	16	CD2	LEU	B	40	-5.421	-54.179	-31.817	1.00	26.69	C
ATOM	17	N	ILE	B	61	-7.271	-56.229	-28.295	1.00	29.38	N
ATOM	18	CA	ILE	B	61	-6.832	-57.616	-28.269	1.00	28.55	C
ATOM	19	C	ILE	B	61	-6.344	-57.855	-26.848	1.00	29.13	C
ATOM	20	O	ILE	B	61	-6.124	-56.906	-26.091	1.00	28.80	O
ATOM	21	CB	ILE	B	61	-5.674	-57.923	-29.258	1.00	28.48	C
ATOM	22	CG1	ILE	B	61	-4.422	-57.126	-28.892	1.00	26.70	C
ATOM	23	CG2	ILE	B	61	-6.123	-57.650	-30.694	1.00	27.65	C
ATOM	24	CD1	ILE	B	61	-3.177	-57.615	-29.638	1.00	27.03	C
ATOM	25	N	ARG	B	62	-6.186	-59.116	-26.473	1.00	29.38	N
ATOM	26	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00	30.76	C
ATOM	27	C	ARG	B	62	-4.274	-59.923	-25.156	1.00	29.32	C
ATOM	28	O	ARG	B	62	-3.933	-60.809	-25.934	1.00	28.65	O
ATOM	29	CB	ARG	B	62	-6.630	-60.447	-24.461	1.00	32.36	C
ATOM	30	CG	ARG	B	62	-6.130	-60.955	-23.114	1.00	35.99	C
ATOM	31	CD	ARG	B	62	-5.438	-59.859	-22.311	1.00	37.86	C
ATOM	32	NE	ARG	B	62	-6.297	-58.718	-22.004	1.00	40.01	N
ATOM	33	CZ	ARG	B	62	-5.840	-57.504	-21.711	1.00	39.09	C
ATOM	34	NH1	ARG	B	62	-4.536	-57.275	-21.690	1.00	39.24	N
ATOM	35	NH2	ARG	B	62	-6.686	-56.518	-21.439	1.00	40.03	N
ATOM	36	N	ILE	B	63	-3.428	-59.342	-24.313	1.00	30.07	N
ATOM	37	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	C
ATOM	38	C	ILE	B	63	-1.623	-59.981	-22.775	1.00	33.08	C
ATOM	39	O	ILE	B	63	-0.444	-59.872	-22.430	1.00	33.21	O
ATOM	40	CB	ILE	B	63	-1.081	-58.745	-24.883	1.00	30.06	C
ATOM	41	CG1	ILE	B	63	-1.143	-57.411	-24.137	1.00	29.94	C
ATOM	42	CG2	ILE	B	63	-1.442	-58.567	-26.353	1.00	30.41	C
ATOM	43	CD1	ILE	B	63	-0.128	-56.384	-24.632	1.00	29.62	C
ATOM	44	N	SER	B	64	-2.603	-60.284	-21.927	1.00	35.38	N
ATOM	45	CA	SER	B	64	-2.356	-60.520	-20.505	1.00	37.51	C
ATOM	46	C	SER	B	64	-1.326	-61.622	-20.311	1.00	37.32	C
ATOM	47	O	SER	B	64	-1.411	-62.682	-20.933	1.00	37.86	O
ATOM	48	CB	SER	B	64	-3.652	-60.912	-19.792	1.00	38.82	C
ATOM	49	OG	SER	B	64	-4.558	-59.823	-19.750	1.00	42.89	O
ATOM	50	N	GLY	B	65	-0.356	-61.370	-19.441	1.00	37.81	N
ATOM	51	CA	GLY	B	65	0.679	-62.355	-19.199	1.00	37.13	C
ATOM	52	C	GLY	B	65	1.798	-62.283	-20.226	1.00	36.76	C
ATOM	53	O	GLY	B	65	2.858	-62.889	-20.038	1.00	37.57	O
ATOM	54	N	LEU	B	66	1.577	-61.539	-21.307	1.00	34.63	N
ATOM	55	CA	LEU	B	66	2.591	-61.413	-22.355	1.00	33.17	C
ATOM	56	C	LEU	B	66	3.414	-60.133	-22.246	1.00	32.72	C
ATOM	57	O	LEU	B	66	4.451	-60.002	-22.893	1.00	33.13	O
ATOM	58	CB	LEU	B	66	1.936	-61.470	-23.735	1.00	32.08	C
ATOM	59	CG	LEU	B	66	1.162	-62.747	-24.061	1.00	32.52	C
ATOM	60	CD1	LEU	B	66	0.563	-62.626	-25.445	1.00	31.38	C

ATOM	61	CD2	LEU	B	66	2.093	-63.957	-23.984	1.00	31.67	C
ATOM	62	N	ARG	B	67	2.953	-59.185	-21.440	1.00	31.54	N
ATOM	63	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	C
ATOM	64	C	ARG	B	67	5.071	-58.142	-20.713	1.00	29.99	C
ATOM	65	O	ARG	B	67	5.294	-59.034	-19.889	1.00	28.67	O
ATOM	66	CB	ARG	B	67	2.888	-56.984	-20.363	1.00	32.28	C
ATOM	67	CG	ARG	B	67	1.540	-56.576	-20.913	1.00	34.65	C
ATOM	68	CD	ARG	B	67	0.926	-55.440	-20.097	1.00	36.69	C
ATOM	69	NE	ARG	B	67	-0.259	-54.889	-20.748	1.00	38.28	N
ATOM	70	CZ	ARG	B	67	-1.425	-55.519	-20.853	1.00	39.05	C
ATOM	71	NH1	ARG	B	67	-1.583	-56.734	-20.341	1.00	39.61	N
ATOM	72	NH2	ARG	B	67	-2.434	-54.935	-21.487	1.00	39.52	N
ATOM	73	N	GLY	B	68	6.014	-57.321	-21.165	1.00	27.75	N
ATOM	74	CA	GLY	B	68	7.380	-57.427	-20.685	1.00	26.79	C
ATOM	75	C	GLY	B	68	8.166	-58.579	-21.280	1.00	25.41	C
ATOM	76	O	GLY	B	68	9.326	-58.779	-20.943	1.00	26.04	O
ATOM	77	N	LYS	B	69	7.546	-59.342	-22.170	1.00	24.55	N
ATOM	78	CA	LYS	B	69	8.238	-60.463	-22.796	1.00	23.93	C
ATOM	79	C	LYS	B	69	8.825	-60.062	-24.142	1.00	23.32	C
ATOM	80	O	LYS	B	69	8.151	-59.404	-24.944	1.00	21.96	O
ATOM	81	CB	LYS	B	69	7.284	-61.641	-23.033	1.00	24.12	C
ATOM	82	CG	LYS	B	69	6.757	-62.360	-21.794	1.00	25.08	C
ATOM	83	CD	LYS	B	69	5.887	-63.553	-22.224	1.00	25.44	C
ATOM	84	CE	LYS	B	69	5.357	-64.358	-21.035	1.00	28.31	C
ATOM	85	NZ	LYS	B	69	6.468	-64.877	-20.175	1.00	29.71	N
ATOM	86	N	GLY	B	70	10.075	-60.470	-24.374	1.00	22.48	N
ATOM	87	CA	GLY	B	70	10.755	-60.229	-25.636	1.00	22.26	C
ATOM	88	C	GLY	B	70	10.308	-61.337	-26.588	1.00	22.17	C
ATOM	89	O	GLY	B	70	9.512	-62.183	-26.195	1.00	21.62	O
ATOM	90	N	ILE	B	71	10.819	-61.373	-27.814	1.00	21.85	N
ATOM	91	CA	ILE	B	71	10.357	-62.386	-28.762	1.00	23.55	C
ATOM	92	C	ILE	B	71	10.616	-63.840	-28.359	1.00	23.88	C
ATOM	93	O	ILE	B	71	9.775	-64.707	-28.592	1.00	21.66	O
ATOM	94	CB	ILE	B	71	10.926	-62.142	-30.181	1.00	23.52	C
ATOM	95	CG1	ILE	B	71	10.264	-63.096	-31.182	1.00	24.18	C
ATOM	96	CG2	ILE	B	71	12.435	-62.375	-30.192	1.00	25.96	C
ATOM	97	CD1	ILE	B	71	8.745	-62.981	-31.263	1.00	25.73	C
ATOM	98	N	LYS	B	72	11.764	-64.119	-27.751	1.00	23.82	N
ATOM	99	CA	LYS	B	72	12.038	-65.491	-27.343	1.00	24.92	C
ATOM	100	C	LYS	B	72	11.068	-65.925	-26.245	1.00	23.73	C
ATOM	101	O	LYS	B	72	10.592	-67.062	-26.245	1.00	24.08	O
ATOM	102	CB	LYS	B	72	13.491	-65.634	-26.875	1.00	26.86	C
ATOM	103	CG	LYS	B	72	14.496	-65.590	-28.019	1.00	31.29	C
ATOM	104	CD	LYS	B	72	15.925	-65.791	-27.518	1.00	36.00	C
ATOM	105	CE	LYS	B	72	16.926	-65.816	-28.671	1.00	38.82	C
ATOM	106	NZ	LYS	B	72	18.342	-65.957	-28.192	1.00	41.21	N
ATOM	107	N	ALA	B	73	10.765	-65.016	-25.322	1.00	21.62	N
ATOM	108	CA	ALA	B	73	9.839	-65.306	-24.233	1.00	21.18	C
ATOM	109	C	ALA	B	73	8.412	-65.454	-24.771	1.00	20.36	C
ATOM	110	O	ALA	B	73	7.619	-66.250	-24.267	1.00	18.97	O
ATOM	111	CB	ALA	B	73	9.895	-64.196	-23.187	1.00	22.25	C
ATOM	112	N	LEU	B	74	8.076	-64.673	-25.791	1.00	20.23	N
ATOM	113	CA	LEU	B	74	6.745	-64.762	-26.387	1.00	19.36	C
ATOM	114	C	LEU	B	74	6.549	-66.110	-27.069	1.00	19.37	C
ATOM	115	O	LEU	B	74	5.539	-66.779	-26.863	1.00	20.01	O
ATOM	116	CB	LEU	B	74	6.540	-63.643	-27.417	1.00	18.42	C
ATOM	117	CG	LEU	B	74	6.422	-62.208	-26.884	1.00	18.80	C
ATOM	118	CD1	LEU	B	74	6.473	-61.197	-28.039	1.00	19.86	C
ATOM	119	CD2	LEU	B	74	5.109	-62.071	-26.104	1.00	19.45	C
ATOM	120	N	ILE	B	75	7.520	-66.507	-27.883	1.00	20.59	N
ATOM	121	CA	ILE	B	75	7.434	-67.768	-28.601	1.00	21.18	C
ATOM	122	C	ILE	B	75	7.488	-68.942	-27.624	1.00	21.20	C
ATOM	123	O	ILE	B	75	7.125	-70.063	-27.979	1.00	21.59	O
ATOM	124	CB	ILE	B	75	8.571	-67.896	-29.641	1.00	22.95	C
ATOM	125	CG1	ILE	B	75	8.598	-66.657	-30.540	1.00	26.82	C
ATOM	126	CG2	ILE	B	75	8.334	-69.108	-30.527	1.00	25.38	C

ATOM	127	CD1	ILE	B	75	7.304	-66.442	-31.327	1.00	28.48	C
ATOM	128	N	ALA	B	76	7.940	-68.680	-26.399	1.00	20.49	N
ATOM	129	CA	ALA	B	76	7.996	-69.726	-25.374	1.00	21.72	C
ATOM	130	C	ALA	B	76	6.624	-69.904	-24.732	1.00	21.54	C
ATOM	131	O	ALA	B	76	6.441	-70.778	-23.875	1.00	20.75	O
ATOM	132	CB	ALA	B	76	9.026	-69.372	-24.305	1.00	21.92	C
ATOM	133	N	ALA	B	77	5.668	-69.066	-25.145	1.00	20.61	N
ATOM	134	CA	ALA	B	77	4.289	-69.121	-24.655	1.00	21.07	C
ATOM	135	C	ALA	B	77	3.383	-69.298	-25.881	1.00	21.69	C
ATOM	136	O	ALA	B	77	2.567	-68.430	-26.199	1.00	21.93	O
ATOM	137	CB	ALA	B	77	3.937	-67.830	-23.924	1.00	20.10	C
ATOM	138	N	PRO	B	78	3.507	-70.446	-26.564	1.00	22.38	N
ATOM	139	CA	PRO	B	78	2.772	-70.846	-27.771	1.00	20.95	C
ATOM	140	C	PRO	B	78	1.278	-70.535	-27.813	1.00	21.19	C
ATOM	141	O	PRO	B	78	0.789	-69.939	-28.776	1.00	19.68	O
ATOM	142	CB	PRO	B	78	3.027	-72.350	-27.861	1.00	22.21	C
ATOM	143	CG	PRO	B	78	4.288	-72.547	-27.117	1.00	24.07	C
ATOM	144	CD	PRO	B	78	4.211	-71.603	-25.976	1.00	21.89	C
ATOM	145	N	LEU	B	79	0.544	-70.961	-26.790	1.00	21.21	N
ATOM	146	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00	21.32	C
ATOM	147	C	LEU	B	79	-1.275	-69.263	-26.707	1.00	21.17	C
ATOM	148	O	LEU	B	79	-2.125	-68.800	-27.481	1.00	20.44	O
ATOM	149	CB	LEU	B	79	-1.569	-71.476	-25.630	1.00	20.99	C
ATOM	150	CG	LEU	B	79	-1.397	-72.988	-25.617	1.00	22.40	C
ATOM	151	CD1	LEU	B	79	-2.504	-73.619	-24.772	1.00	22.01	C
ATOM	152	CD2	LEU	B	79	-1.438	-73.521	-27.021	1.00	23.82	C
ATOM	153	N	ARG	B	80	-0.656	-68.529	-25.788	1.00	20.91	N
ATOM	154	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00	21.30	C
ATOM	155	C	ARG	B	80	-0.526	-66.233	-26.790	1.00	21.29	C
ATOM	156	O	ARG	B	80	-1.278	-65.355	-27.223	1.00	21.47	O
ATOM	157	CB	ARG	B	80	-0.444	-66.583	-24.312	1.00	22.12	C
ATOM	158	CG	ARG	B	80	-1.286	-67.051	-23.118	1.00	24.03	C
ATOM	159	CD	ARG	B	80	-0.610	-66.738	-21.807	1.00	23.42	C
ATOM	160	NE	ARG	B	80	0.581	-67.556	-21.610	1.00	24.59	N
ATOM	161	CZ	ARG	B	80	1.466	-67.351	-20.642	1.00	26.08	C
ATOM	162	NH1	ARG	B	80	1.290	-66.349	-19.787	1.00	26.92	N
ATOM	163	NH2	ARG	B	80	2.514	-68.152	-20.519	1.00	27.22	N
ATOM	164	N	ILE	B	81	0.683	-66.448	-27.303	1.00	19.29	N
ATOM	165	CA	ILE	B	81	1.113	-65.621	-28.421	1.00	19.47	C
ATOM	166	C	ILE	B	81	0.256	-65.937	-29.654	1.00	18.99	C
ATOM	167	O	ILE	B	81	-0.149	-65.028	-30.378	1.00	19.38	O
ATOM	168	CB	ILE	B	81	2.639	-65.793	-28.730	1.00	17.92	C
ATOM	169	CG1	ILE	B	81	3.067	-64.753	-29.769	1.00	18.63	C
ATOM	170	CG2	ILE	B	81	2.949	-67.200	-29.206	1.00	17.33	C
ATOM	171	CD1	ILE	B	81	2.746	-63.318	-29.346	1.00	17.46	C
ATOM	172	N	PHE	B	82	-0.056	-67.211	-29.880	1.00	19.39	N
ATOM	173	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00	19.15	C
ATOM	174	C	PHE	B	82	-2.250	-66.931	-30.959	1.00	19.94	C
ATOM	175	O	PHE	B	82	-2.777	-66.444	-31.970	1.00	19.64	O
ATOM	176	CB	PHE	B	82	-1.057	-69.103	-31.136	1.00	19.27	C
ATOM	177	CG	PHE	B	82	-1.811	-69.548	-32.368	1.00	19.87	C
ATOM	178	CD1	PHE	B	82	-1.180	-69.602	-33.603	1.00	20.87	C
ATOM	179	CD2	PHE	B	82	-3.154	-69.898	-32.289	1.00	21.11	C
ATOM	180	CE1	PHE	B	82	-1.872	-70.002	-34.753	1.00	21.20	C
ATOM	181	CE2	PHE	B	82	-3.857	-70.297	-33.429	1.00	22.26	C
ATOM	182	CZ	PHE	B	82	-3.212	-70.349	-34.663	1.00	22.14	C
ATOM	183	N	ASN	B	83	-2.832	-66.923	-29.764	1.00	19.29	N
ATOM	184	CA	ASN	B	83	-4.150	-66.332	-29.577	1.00	20.90	C
ATOM	185	C	ASN	B	83	-4.178	-64.821	-29.812	1.00	20.83	C
ATOM	186	O	ASN	B	83	-5.086	-64.316	-30.472	1.00	21.92	O
ATOM	187	CB	ASN	B	83	-4.693	-66.641	-28.178	1.00	20.55	C
ATOM	188	CG	ASN	B	83	-6.158	-66.244	-28.028	1.00	22.79	C
ATOM	189	OD1	ASN	B	83	-6.505	-65.374	-27.229	1.00	25.14	O
ATOM	190	ND2	ASN	B	83	-7.018	-66.877	-28.807	1.00	20.47	N
ATOM	191	N	ALA	B	84	-3.203	-64.092	-29.275	1.00	19.74	N
ATOM	192	CA	ALA	B	84	-3.177	-62.647	-29.484	1.00	19.30	C

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ATOM    193  C   ALA B  84      -2.967 -62.380 -30.981  1.00 19.94      C
ATOM    194  O   ALA B  84      -3.561 -61.459 -31.552  1.00 19.69      O
ATOM    195  CB  ALA B  84      -2.060 -62.008 -28.662  1.00 18.59      C
ATOM    196  N   TRP B  85      -2.118 -63.197 -31.603  1.00 19.77      N
ATOM    197  CA  TRP B  85      -1.820 -63.111 -33.032  1.00 20.56      C
ATOM    198  C   TRP B  85      -3.090 -63.354 -33.865  1.00 21.76      C
ATOM    199  O   TRP B  85      -3.339 -62.658 -34.859  1.00 20.40      O
ATOM    200  CB  TRP B  85      -0.754 -64.148 -33.396  1.00 21.46      C
ATOM    201  CG  TRP B  85      -0.365 -64.167 -34.856  1.00 23.00      C
ATOM    202  CD1 TRP B  85       0.301 -63.189 -35.548  1.00 23.17      C
ATOM    203  CD2 TRP B  85      -0.588 -65.232 -35.785  1.00 23.69      C
ATOM    204  NE1 TRP B  85       0.509 -63.585 -36.848  1.00 24.28      N
ATOM    205  CE2 TRP B  85      -0.024 -64.835 -37.022  1.00 24.14      C
ATOM    206  CE3 TRP B  85      -1.206 -66.486 -35.693  1.00 24.79      C
ATOM    207  CZ2 TRP B  85      -0.060 -65.650 -38.160  1.00 24.90      C
ATOM    208  CZ3 TRP B  85      -1.243 -67.299 -36.827  1.00 25.45      C
ATOM    209  CH2 TRP B  85      -0.671 -66.875 -38.045  1.00 25.15      C
ATOM    210  N   ARG B  86      -3.885 -64.346 -33.467  1.00 22.03      N
ATOM    211  CA  ARG B  86      -5.140 -64.660 -34.166  1.00 23.28      C
ATOM    212  C   ARG B  86      -6.151 -63.517 -34.007  1.00 22.98      C
ATOM    213  O   ARG B  86      -6.890 -63.195 -34.942  1.00 21.37      O
ATOM    214  CB  ARG B  86      -5.754 -65.965 -33.623  1.00 24.72      C
ATOM    215  CG  ARG B  86      -4.999 -67.236 -34.021  1.00 27.21      C
ATOM    216  CD  ARG B  86      -5.368 -67.725 -35.418  1.00 29.60      C
ATOM    217  NE  ARG B  86      -6.626 -68.477 -35.422  1.00 31.45      N
ATOM    218  CZ  ARG B  86      -7.185 -69.004 -36.508  1.00 31.37      C
ATOM    219  NH1 ARG B  86      -6.607 -68.862 -37.696  1.00 32.19      N
ATOM    220  NH2 ARG B  86      -8.314 -69.694 -36.405  1.00 31.39      N
ATOM    221  N   GLN B  87      -6.190 -62.916 -32.821  1.00 22.90      N
ATOM    222  CA  GLN B  87      -7.101 -61.802 -32.567  1.00 24.07      C
ATOM    223  C   GLN B  87      -6.738 -60.618 -33.457  1.00 23.85      C
ATOM    224  O   GLN B  87      -7.613 -60.012 -34.077  1.00 24.02      O
ATOM    225  CB  GLN B  87      -7.046 -61.382 -31.097  1.00 24.33      C
ATOM    226  CG  GLN B  87      -7.873 -62.280 -30.187  1.00 27.24      C
ATOM    227  CD  GLN B  87      -7.720 -61.943 -28.723  1.00 28.81      C
ATOM    228  OE1 GLN B  87      -8.567 -62.296 -27.908  1.00 33.25      O
ATOM    229  NE2 GLN B  87      -6.632 -61.275 -28.375  1.00 29.95      N
ATOM    230  N   ALA B  88      -5.449 -60.293 -33.521  1.00 23.39      N
ATOM    231  CA  ALA B  88      -4.996 -59.183 -34.355  1.00 23.78      C
ATOM    232  C   ALA B  88      -5.257 -59.485 -35.831  1.00 24.73      C
ATOM    233  O   ALA B  88      -5.655 -58.595 -36.592  1.00 24.72      O
ATOM    234  CB  ALA B  88      -3.508 -58.909 -34.116  1.00 23.33      C
ATOM    235  N   ARG B  89      -5.038 -60.735 -36.244  1.00 24.26      N
ATOM    236  CA  ARG B  89      -5.285 -61.111 -37.636  1.00 24.94      C
ATOM    237  C   ARG B  89      -6.752 -60.909 -38.013  1.00 25.29      C
ATOM    238  O   ARG B  89      -7.056 -60.420 -39.104  1.00 24.27      O
ATOM    239  CB  ARG B  89      -4.904 -62.575 -37.893  1.00 25.14      C
ATOM    240  CG  ARG B  89      -3.461 -62.774 -38.353  1.00 24.54      C
ATOM    241  CD  ARG B  89      -3.142 -64.253 -38.510  1.00 25.50      C
ATOM    242  NE  ARG B  89      -3.809 -64.901 -39.641  1.00 24.93      N
ATOM    243  CZ  ARG B  89      -3.329 -64.930 -40.882  1.00 25.90      C
ATOM    244  NH1 ARG B  89      -2.178 -64.336 -41.170  1.00 25.98      N
ATOM    245  NH2 ARG B  89      -3.979 -65.596 -41.831  1.00 26.36      N
ATOM    246  N   GLY B 105       5.583 -50.364 -27.741  1.00 23.01      N
ATOM    247  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54      C
ATOM    248  C   GLY B 105       4.358 -52.380 -27.078  1.00 23.17      C
ATOM    249  O   GLY B 105       4.449 -52.844 -28.214  1.00 22.69      O
ATOM    250  N   TYR B 106       4.018 -53.118 -26.026  1.00 22.87      N
ATOM    251  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37      C
ATOM    252  C   TYR B 106       2.719 -55.018 -27.100  1.00 20.52      C
ATOM    253  O   TYR B 106       2.867 -56.052 -27.746  1.00 20.50      O
ATOM    254  CB  TYR B 106       3.632 -55.181 -24.774  1.00 25.08      C
ATOM    255  CG  TYR B 106       4.864 -55.008 -23.929  1.00 28.19      C
ATOM    256  CD1 TYR B 106       4.869 -54.153 -22.830  1.00 31.96      C
ATOM    257  CD2 TYR B 106       6.058 -55.631 -24.282  1.00 31.27      C
ATOM    258  CE1 TYR B 106       6.043 -53.915 -22.108  1.00 33.13      C
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ATOM    259  CE2 TYR B 106       7.234 -55.400 -23.569  1.00 32.27      C
ATOM    260  CZ  TYR B 106       7.219 -54.541 -22.487  1.00 33.19      C
ATOM    261  OH  TYR B 106       8.388 -54.291 -21.802  1.00 35.95      O
ATOM    262  N   VAL B 107       1.628 -54.270 -27.205  1.00 19.06      N
ATOM    263  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06      C
ATOM    264  C   VAL B 107       1.015 -54.743 -29.559  1.00 17.45      C
ATOM    265  O   VAL B 107       0.502 -55.536 -30.346  1.00 16.99      O
ATOM    266  CB  VAL B 107      -0.690 -53.774 -27.978  1.00 20.95      C
ATOM    267  CG1 VAL B 107      -0.407 -52.407 -28.589  1.00 21.39      C
ATOM    268  CG2 VAL B 107      -1.879 -54.433 -28.658  1.00 21.30      C
ATOM    269  N   SER B 108       1.991 -53.916 -29.918  1.00 17.96      N
ATOM    270  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67      C
ATOM    271  C   SER B 108       3.197 -55.187 -31.694  1.00 20.38      C
ATOM    272  O   SER B 108       3.385 -55.449 -32.884  1.00 21.25      O
ATOM    273  CB  SER B 108       3.424 -52.691 -31.508  1.00 19.56      C
ATOM    274  OG  SER B 108       4.666 -52.824 -30.837  1.00 19.63      O
ATOM    275  N   GLY B 109       3.595 -55.995 -30.710  1.00 19.59      N
ATOM    276  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03      C
ATOM    277  C   GLY B 109       3.311 -58.170 -31.792  1.00 19.61      C
ATOM    278  O   GLY B 109       3.579 -58.517 -32.940  1.00 19.24      O
ATOM    279  N   PRO B 110       2.206 -58.606 -31.173  1.00 19.20      N
ATOM    280  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99      C
ATOM    281  C   PRO B 110       0.651 -58.761 -33.075  1.00 19.22      C
ATOM    282  O   PRO B 110       0.406 -59.371 -34.116  1.00 17.13      O
ATOM    283  CB  PRO B 110       0.198 -59.737 -30.778  1.00 20.41      C
ATOM    284  CG  PRO B 110       0.998 -59.720 -29.515  1.00 19.81      C
ATOM    285  CD  PRO B 110       1.914 -58.528 -29.729  1.00 19.94      C
ATOM    286  N   GLY B 111       0.407 -57.462 -32.927  1.00 19.03      N
ATOM    287  CA  GLY B 111      -0.160 -56.702 -34.025  1.00 19.60      C
ATOM    288  C   GLY B 111       0.764 -56.714 -35.226  1.00 19.59      C
ATOM    289  O   GLY B 111       0.330 -56.979 -36.339  1.00 21.10      O
ATOM    290  N   GLY B 112       2.043 -56.429 -34.995  1.00 19.78      N
ATOM    291  CA  GLY B 112       3.014 -56.417 -36.074  1.00 19.97      C
ATOM    292  C   GLY B 112       3.147 -57.783 -36.724  1.00 20.43      C
ATOM    293  O   GLY B 112       3.233 -57.896 -37.949  1.00 19.94      O
ATOM    294  N   LEU B 113       3.167 -58.828 -35.903  1.00 19.26      N
ATOM    295  CA  LEU B 113       3.265 -60.184 -36.429  1.00 19.49      C
ATOM    296  C   LEU B 113       2.040 -60.521 -37.274  1.00 18.73      C
ATOM    297  O   LEU B 113       2.143 -61.252 -38.255  1.00 18.44      O
ATOM    298  CB  LEU B 113       3.405 -61.198 -35.289  1.00 18.38      C
ATOM    299  CG  LEU B 113       4.777 -61.270 -34.605  1.00 20.59      C
ATOM    300  CD1 LEU B 113       4.656 -62.059 -33.311  1.00 20.01      C
ATOM    301  CD2 LEU B 113       5.794 -61.914 -35.538  1.00 20.23      C
ATOM    302  N   ALA B 114       0.875 -60.010 -36.892  1.00 18.96      N
ATOM    303  CA  ALA B 114      -0.334 -60.292 -37.661  1.00 18.70      C
ATOM    304  C   ALA B 114      -0.288 -59.578 -39.019  1.00 19.30      C
ATOM    305  O   ALA B 114      -0.602 -60.167 -40.052  1.00 20.62      O
ATOM    306  CB  ALA B 114      -1.562 -59.855 -36.889  1.00 16.45      C
ATOM    307  N   ALA B 115       0.082 -58.303 -39.000  1.00 20.57      N
ATOM    308  CA  ALA B 115       0.167 -57.516 -40.229  1.00 21.84      C
ATOM    309  C   ALA B 115       1.140 -58.192 -41.189  1.00 21.58      C
ATOM    310  O   ALA B 115       0.815 -58.464 -42.345  1.00 22.14      O
ATOM    311  CB  ALA B 115       0.636 -56.108 -39.911  1.00 19.85      C
ATOM    312  N   TRP B 116       2.334 -58.476 -40.688  1.00 22.12      N
ATOM    313  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22      C
ATOM    314  C   TRP B 116       2.871 -60.434 -42.123  1.00 23.55      C
ATOM    315  O   TRP B 116       3.048 -60.643 -43.329  1.00 22.19      O
ATOM    316  CB  TRP B 116       4.584 -59.367 -40.579  1.00 26.08      C
ATOM    317  CG  TRP B 116       5.699 -60.136 -41.204  1.00 27.40      C
ATOM    318  CD1 TRP B 116       6.473 -59.761 -42.271  1.00 28.30      C
ATOM    319  CD2 TRP B 116       6.168 -61.418 -40.793  1.00 28.77      C
ATOM    320  NE1 TRP B 116       7.401 -60.742 -42.547  1.00 29.04      N
ATOM    321  CE2 TRP B 116       7.234 -61.771 -41.655  1.00 30.37      C
ATOM    322  CE3 TRP B 116       5.794 -62.308 -39.778  1.00 30.49      C
ATOM    323  CZ2 TRP B 116       7.929 -62.981 -41.529  1.00 31.08      C
ATOM    324  CZ3 TRP B 116       6.485 -63.510 -39.653  1.00 31.85      C
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ATOM	325	CH2	TRP	B	116	7.541	-63.834	-40.527	1.00	32.27	C
ATOM	326	N	SER	B	117	2.231	-61.304	-41.338	1.00	21.35	N
ATOM	327	CA	SER	B	117	1.735	-62.573	-41.873	1.00	22.61	C
ATOM	328	C	SER	B	117	0.665	-62.383	-42.940	1.00	23.56	C
ATOM	329	O	SER	B	117	0.463	-63.262	-43.780	1.00	23.11	O
ATOM	330	CB	SER	B	117	1.167	-63.462	-40.756	1.00	20.72	C
ATOM	331	OG	SER	B	117	0.010	-62.889	-40.169	1.00	22.72	O
ATOM	332	N	LEU	B	133	11.788	-52.846	-25.860	1.00	23.38	N
ATOM	333	CA	LEU	B	133	11.903	-54.293	-26.020	1.00	24.54	C
ATOM	334	C	LEU	B	133	11.209	-54.833	-27.276	1.00	22.84	C
ATOM	335	O	LEU	B	133	11.784	-55.619	-28.027	1.00	21.86	O
ATOM	336	CB	LEU	B	133	11.328	-54.996	-24.786	1.00	25.48	C
ATOM	337	CG	LEU	B	133	11.388	-56.527	-24.780	1.00	27.50	C
ATOM	338	CD1	LEU	B	133	12.840	-56.984	-24.866	1.00	28.69	C
ATOM	339	CD2	LEU	B	133	10.735	-57.059	-23.509	1.00	28.04	C
ATOM	340	N	THR	B	134	9.975	-54.401	-27.499	1.00	21.72	N
ATOM	341	CA	THR	B	134	9.202	-54.860	-28.639	1.00	21.22	C
ATOM	342	C	THR	B	134	9.693	-54.326	-29.986	1.00	20.62	C
ATOM	343	O	THR	B	134	9.843	-55.091	-30.932	1.00	20.33	O
ATOM	344	CB	THR	B	134	7.716	-54.509	-28.449	1.00	20.99	C
ATOM	345	OG1	THR	B	134	7.257	-55.075	-27.210	1.00	20.94	O
ATOM	346	CG2	THR	B	134	6.872	-55.073	-29.600	1.00	20.64	C
ATOM	3608	N	LYS	B	136	12.595	-53.366	-30.809	1.00	21.46	N
ATOM	3609	CA	LYS	B	136	13.886	-53.949	-31.144	1.00	22.79	C
ATOM	3610	CB	LYS	B	136	14.713	-54.196	-29.879	1.00	24.70	C
ATOM	3611	CG	LYS	B	136	16.183	-54.424	-30.178	1.00	27.75	C
ATOM	3612	CD	LYS	B	136	16.998	-54.494	-28.902	1.00	30.17	C
ATOM	3613	CE	LYS	B	136	18.479	-54.671	-29.203	1.00	32.33	C
ATOM	3614	NZ	LYS	B	136	19.278	-54.641	-27.944	1.00	33.37	N
ATOM	3615	C	LYS	B	136	13.793	-55.229	-31.966	1.00	23.46	C
ATOM	3616	O	LYS	B	136	14.561	-55.407	-32.912	1.00	23.71	O
ATOM	347	N	TRP	B	137	12.868	-56.127	-31.633	1.00	21.78	N
ATOM	348	CA	TRP	B	137	12.753	-57.345	-32.424	1.00	22.06	C
ATOM	349	C	TRP	B	137	11.768	-57.202	-33.574	1.00	21.75	C
ATOM	350	O	TRP	B	137	11.936	-57.822	-34.623	1.00	21.76	O
ATOM	351	CB	TRP	B	137	12.361	-58.552	-31.553	1.00	21.20	C
ATOM	352	CG	TRP	B	137	10.990	-58.525	-30.922	1.00	20.23	C
ATOM	353	CD1	TRP	B	137	10.696	-58.231	-29.618	1.00	19.62	C
ATOM	354	CD2	TRP	B	137	9.748	-58.877	-31.544	1.00	18.68	C
ATOM	355	NE1	TRP	B	137	9.349	-58.385	-29.390	1.00	19.31	N
ATOM	356	CE2	TRP	B	137	8.743	-58.780	-30.555	1.00	18.97	C
ATOM	357	CE3	TRP	B	137	9.383	-59.270	-32.840	1.00	19.75	C
ATOM	358	CZ2	TRP	B	137	7.401	-59.058	-30.821	1.00	18.18	C
ATOM	359	CZ3	TRP	B	137	8.046	-59.549	-33.107	1.00	18.87	C
ATOM	360	CH2	TRP	B	137	7.072	-59.440	-32.099	1.00	18.94	C
ATOM	361	N	LEU	B	138	10.741	-56.381	-33.386	1.00	21.61	N
ATOM	362	CA	LEU	B	138	9.744	-56.188	-34.431	1.00	23.15	C
ATOM	363	C	LEU	B	138	10.384	-55.558	-35.676	1.00	23.07	C
ATOM	364	O	LEU	B	138	9.958	-55.801	-36.809	1.00	22.68	O
ATOM	365	CB	LEU	B	138	8.618	-55.305	-33.886	1.00	23.87	C
ATOM	366	CG	LEU	B	138	7.312	-55.155	-34.664	1.00	26.48	C
ATOM	367	CD1	LEU	B	138	6.672	-56.508	-34.915	1.00	25.34	C
ATOM	368	CD2	LEU	B	138	6.383	-54.267	-33.851	1.00	25.90	C
ATOM	3644	N	LYS	B	140	12.801	-56.332	-37.241	1.00	27.38	N
ATOM	3645	CA	LYS	B	140	13.279	-57.337	-38.182	1.00	28.05	C
ATOM	3646	CB	LYS	B	140	13.893	-58.501	-37.401	1.00	29.91	C
ATOM	3647	CG	LYS	B	140	15.134	-58.057	-36.635	1.00	31.62	C
ATOM	3648	CD	LYS	B	140	15.719	-59.149	-35.757	1.00	33.53	C
ATOM	3649	CE	LYS	B	140	16.974	-58.634	-35.055	1.00	34.46	C
ATOM	3650	NZ	LYS	B	140	17.692	-59.713	-34.320	1.00	36.17	N
ATOM	3651	C	LYS	B	140	12.254	-57.833	-39.212	1.00	27.83	C
ATOM	3652	O	LYS	B	140	12.602	-58.562	-40.142	1.00	27.80	O
ATOM	369	N	ILE	B	141	10.992	-57.445	-39.052	1.00	26.40	N
ATOM	370	CA	ILE	B	141	9.963	-57.818	-40.016	1.00	26.09	C
ATOM	371	C	ILE	B	141	9.316	-56.542	-40.530	1.00	25.81	C
ATOM	372	O	ILE	B	141	8.353	-56.586	-41.305	1.00	26.10	O

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ATOM    373  CB  ILE B 141       8.854 -58.721 -39.405  1.00 26.39      C
ATOM    374  CG1 ILE B 141       8.298 -58.092 -38.127  1.00 26.45      C
ATOM    375  CG2 ILE B 141       9.401 -60.118 -39.145  1.00 28.33      C
ATOM    376  CD1 ILE B 141       7.136 -58.845 -37.549  1.00 26.95      C
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The following examples are presented for purposes of illustration only and are not intended to limit the scope of the invention in any way.

EXAMPLE 1

This example describes the crystallization of the *E. coli* MurG protein and the determination of the coordinates of the three-dimensional crystal structure. This example also describes the identification of the donor nucleotide binding site, the acceptor binding site and the membrane association site of the MurG protein.

Abstract

The 1.9 Å X-ray structure of a membrane-associated glycosyltransferase involved in peptidoglycan biosynthesis is reported. This enzyme, MurG, contains two ?/? open sheet domains separated by a deep cleft. The C-terminal domain contains the UDP-GlcNAc binding site while the N-terminal domain contains the acceptor binding site and likely membrane association site. Combined with sequence data from other MurG homologs, this structure provides insight into the residues that are important in substrate binding and catalysis. We have also noted that a conserved region found in many UDP-sugar transferases maps to a ?/?/?/? supersecondary structural motif in the donor binding region of MurG, an observation that is be helpful in glycosyltransferase structure prediction.

Methods

Crystallization

E. coli MurG containing a C-terminal LEHHHHHH sequence was purified as described(Ha *et al.*, 1999) and concentrated to 10 mg ml^{-1} in 20 mM Tris-HCl, pH 7.9/ 150 mM NaCl/ 50 mM EDTA. The protein concentrate was mixed with UDP-GlcNAc

in a 1:3 molar ratio. Crystals were grown at room temperature using the hanging-drop vapor-diffusion method by mixing equal volumes of protein with reservoir solution (0.1 M NaMES, pH 6.5/ 0.96 M $(NH_4)_2SO_4$/ 0.4% Triton X-100/ 10 mM DTT). Triclinic crystals with a typical size of 0.2 mm X 0.1 mm X 0.1 mm grew within a week. The crystals belong to the P1 space group, with two molecules per asymmetric unit. The cell dimensions are a=60.613 Å, b=66.356 Å, c=67.902 Å, ?=64.294, ?=83.520, ????????????

Data collection and processing

All data sets were collected at 100 K on previously flash frozen crystals. Crystals were equilibrated in a cryoprotectant buffer with 0.1 M NaMES, pH 6.5, 1.44 M $(NH_4)_2SO_4$, 0.4% Triton X-100, and 20% glycerol. Heavy-atom soaks were carried out in the same buffer containing one of the following heavy-atom solutions: 2 mM $HgCl_2$, 1 mM $(NH_4)_2WS_4$, 1 mM $(NH_4)_2OsBr_6$. Crystals were flash-frozen in liquid nitrogen. $HgCl_2$ (form A derivative) and $(NH_4)_2OsBr_6$ derivative data were collected at an R-AXISIIC imaging plate detector mounted on a Rigaku 200HB generator. Native, $HgCl_2$ (form B derivative), and $(NH_4)_2WS_4$ derivative diffraction data were collected at beam-line BioCARS-14B at the Advanced Photon Source, at wavelengths 1.0092 Å, 0.9900 Å and 1.2147 Å respectively. Collection of data on the $HgCl_2$ derivative was initially designed for MAD phasing; however, the mercury derivative proved to be unstable to X-rays, and after a two-hour exposure to synchrotron radiation the form A derivative metamorphosed into a different mercury derivative (form B) that was suitable for MIR phasing. All the data were reduced using DENZO and SCALEPACK (Otwinowski & Minor, 1997), and processed with CCP4 programs (CCP4, 1994).

Structure determination and refinement

The structure was solved by multiple isomorphous replacement combined with anomalous scattering of mercuric derivatives (Table 1). Initial MIR phases calculated with program MLPHARE had a mean figure of merit of 0.44 to 2.5 Å, and were improved by solvent flattening and histogram matching using DM. An MIR map was generated which had continuous electron density for most regions of the protein. A model was built with the program O (Jones *et al.*, 1991), and the structure was refined against 1.9 Å data using energy minimization, simulated annealing and B-factor

refinement with the program CNS (Brunger *et al.*, 1998). The N-terminal six residues and the C-terminal His-tag had no electron density and were not included in this model. There was no electron density for UDP-GlcNAc.

Results and discussion

Overall fold

The crystal structure of *E. coli* MurG was solved by a combination of multiple isomorphous replacement and anomalous scattering, and refined to 1.9 Å resolution (Table 1).

Table 1. Summary of crystallographic and refinement data

Data set	Native	$HgCl_2$ (form A derivative)	$HgCl_2$ (form B derivative)	$(NH_4)_2WS_4$	$(NH_4)_2OsBr$
Resolution (Å)	1.9	2.0	1.9	2.4	2.3
Observations	288,150	101,913	245,320	44,366	106,606
Unique reflections	65,567	53,391	65,581	27,950	36,443
R_{sym}[1] (last shell)	0.032 (0.187)	0.043 (0.200)	0.042 (0.296)	0.031 (0.080)	0.056 (0.30
I/? (last shell)	41.9 (7.0)	20.4 (2.9)	29.0 (3.7)	24.6 (8.2)	19.6 (2.5)
Completeness (last shell)	97.7% (96.4%)	91.4% (66.6%)	97.4% (94.0%)	83.8% (62.0%)	94.3% (78.6
MIR analysis (40.0 - 2.5 Å)					
Mean isomorphous difference[2]		0.163	0.130	0.068	0.134
Phasing power[3] (last shell)		1.09 (0.73)	0.57 (0.50)	0.61 (0.24)	0.61 (0.58
R_{cullis} [4] (last shell)		0.81 (0.91)	0.94 (0.96)	0.92 (0.99)	0.94 (0.95
Anomalous R_{cullis} [4] (last shell)		0.96 (1.00)	0.95 (1.00)		

Refinement statistics			
Resolution	40.0 - 1.9 Å	R. m. s. d.[7]	
Reflections (|F| > 2?)	61,989	Bonds (Å)	0.006
Protein atoms (a. u.)	5,280	Angles (°)	1.29
Water Atoms	298		
Sulfate groups	1	Ramachandran plot[8]	
R-factor[5]	22.0%	Residues in most favored region	94.6%
R-free[6]	24.7%	Residues in additional allowed region	5.4%

[1] R_{sym} = ?| I_i - <I> | / ?I_i, where I_i is the intensity of a reflection, and <I> is the average intensity of that reflection.

[2] Mean isomorphous difference = ? |F_{PH} - F_P| / ?F_{PH}, where F_{PH} and F_P are the derivative and native structure factors respectively.

[3] Phasing power is the ratio of the mean calculated derivative structure factor to the mean lack of closure error.

[4] R_{cullis} is the mean residual lack of closure error divided by the dispersive or anomalous difference.

[5] R-factor = ? | |F_{obs}| - |F_{calc}| | / ? |F_{obs}|

[6] R-free is the R-factor calculated using 10% of the reflection data chosen randomly and omitted from the start of refinement.

[7] R. m. s. d., root-mean-square deviations from ideal bond lengths and bond angles.

[8] Calculated with program PROCHECK.

The structure consists of two domains separated by a deep cleft (Fig. 2a). Both domains exhibit an ?/? open-sheet structure and have high structural homology despite minimal sequence homology (RMSD = 2.02 over 85 aligned C? atoms). The N-domain includes residues 7-163 and 341-357, and contains seven parallel ?-strands and six ?-helices, the last of which originates in the C-domain (Fig. 2b). The C-domain comprises residues 164-340 and contains six parallel ?-strands and eight ?-helices, including one irregular bipartite helix (?-link) that connects the N-domain to the first ?-strand of the C-domain. The ?-strands in both domains are ordered as for a typical Rossman fold. The N- and C-domains are joined by a short linker between the seventh ?-strand of the N-domain and the ?-link of the C-domain. This inter-domain linker and the peptide segment that joins the last helix of the C-domain to the last helix of the N-domain define the floor of the cleft between the two domains. The cleft itself is about 20 Å deep and 18 Å across at its widest point. Contacts < 4 Å across the cleft are limited primarily to interactions between residues from C-?5 to the loop connecting N-?5 to N-?5.

The ?/? open-sheet motif (Rossman fold) adopted by both the N- and C-domains of MurG is characteristic of domains that bind nucleotides (Branden & Tooze, 1998). Classical Rossman domains typically contain at least one conserved glycine rich motif, with the consensus sequence GXGXXG, located at a turn between the carboxyl end of one ?-strand and the amino terminus of the adjacent ?-helix (Baker *et al.*, 1992). This motif is involved in binding the negatively charged phosphates (Carugo & Argos, 1997). There are three glycine rich loops (G loops) in *E. coli* MurG (Fig. 3a) that may be variants on the phosphate binding loops found in other dinucleotide binding proteins (see below).

Sequence homology

Amino acid sequences for eighteen MurG homologs are now available. The sequence similarity between *E. coli* MurG and homologs from other bacterial strains ranges from less than 30% to more than 90% depending on the evolutionary relationship between the organisms. In all MurG homologs, however, there are several invariant residues. Fig. 3a shows a sequence alignment for a subset of MurG homologs with the invariant and

highly conserved residues indicated. These residues, which include the three G loops, have been highlighted in the *E. coli* MurG structure (Fig. 3b). Almost all of the invariant residues are located at or near the cleft between the two domains. Two of the G loops are found in the N domain (between N-?1/N-?1 and N-?4/N-?4) and one is found in the C-domain (between C-?1/C-?1). The strict conservation of the highlighted residues among different bacterial strains, and their location as determined from the *E. coli* MurG structure, implicates them in substrate binding and catalytic activity.

Structural homology reveals the donor binding site

The three-dimensional backbone structure of *E. coli* MurG was compared to known protein structures, including the three other NDP-glycosyltransferase structures that have been reported (Charnok & Davies, 1999; Gastinel *et al.*, 1999; Vrielink *et al.*, 1994). The C-terminal domain was found to have significant structural homology (RMSD= 2.218 Å for 89 aligned C? atoms) to the C-terminal domain of phage T4 ?-glucosyltransferase (BGT), an enzyme that catalyzes the glucosylation of hydroxymethyl-cytosines in duplex DNA. A co-crystal structure of BGT with UDP bound in the C-terminal domain reveals the topology of the UDP binding pocket and also shows important contacts to the nucleotide (Moréra *et al.*, 1999; Vrielink *et al.*, 1994). These contacts include: a) hydrogen bonds from the backbone amide of I238 to the N3 and O4 positions of the base; b) hydrogen bonds between the carboxyl side chain of E272 and the O2' and O3' hydroxyls of the ribose ring; and c) contacts from a GGS motif in the loop following the first ?-strand of the C domain to the alpha phosphate of UDP. The structurally homologous C-domain of MurG contains a topologically similar pocket (Fig. 4a). Furthermore, even though the two domains share only 11% sequence identity overall, there are identical residues in the same spatial location in *E. coli* MurG and in BGT. Based on this comparison, we have concluded that the C-domain of *E. coli* MurG is the UDP-GlcNAc binding site.

We have docked UDP-GlcNAc into the C-domain of *E. coli* MurG using the information on how UDP binds to BGT as a guide. As shown in Figure 4b, the uracil is held in place by contacts from the N3 and O4 atoms to the backbone amide of I245. The O2' and O3' hydroxyls on the ribose sugar are within hydrogen bonding distance of the invariant glutamate residue (E269) in the middle of helix C-?4. The conserved GGS

motif in G loop 3 is positioned to contact the alpha phosphate. When these contacts are made, the UDP-GlcNAc substrate fits nicely into a pocket in the C-domain, where it is surrounded by many of the invariant residues identified through sequence analysis of other MurG homologs. It is possible to propose roles for some of these invariant residues from the model. For example, the side chain of R261 can be rotated to contact the second phosphate; this contact may help explain why UDP binds significantly better to MurG than UMP. We propose that R261 plays an important role in catalysis by stabilizing the UDP leaving group via electrostatic interactions. The side chain of Q289 is within hydrogen bonding distance of the C4 hydroxyl of the GlcNAc sugar. This contact may explain why MurG can discriminate between UDP-GlcNAc and its C4 axial isomer, UDP-GalNAc (Ha *et al.*, 1999).

The acceptor binding site

Structural considerations suggest that the primary acceptor binding site is located in the N-terminal domain of MurG. This domain contains three highly conserved regions, two of which are glycine-rich loops that face the cleft (Fig 3a and 4c). These G loops are reminiscent of the phosphate binding loops found in other nucleotide binding proteins, and are most likely involved in binding to the diphosphate on Lipid I. The N-termini of the helices following each G loop form opposite walls of a small pocket between the G loops. The helix dipoles create a positively charged electrostatic field in the pocket that can stabilize the negative charged diphosphates. When the diphosphate of the acceptor is anchored in the pocket created by the G-loops, the MurNAc sugar emerges into the cleft between domains and the C4 hydroxyl can be directed towards the anomeric carbon of the GlcNAc for attack on the face opposite the UDP leaving group. The third conserved region in the N domain spans the loop from the end of N-?5 to the middle of N-?5. Kinetic analysis of mutants is required to evaluate the roles of these residues (Ha *et al.*, 1999; Men *et al.*, 1998).

Proposed membrane association site

MurG associates with the cytoplasmic surface of bacterial membranes where it couples a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG structure shows that there is a hydrophobic patch consisting of residues

I75, L79, F82, W85 and W116 in the N-domain, which is surrounded by basic residues (K72, K140, K69, R80, R86, R89). We propose that this is the membrane association site and that association involves both hydrophobic and electrostatic interactions with the negatively charged bacterial membrane. The location of this patch in MurG is also consistent with the proposed acceptor binding site: membrane association at this patch would bring the two N-terminal G loops close to the membrane surface where the diphosphate portion of the acceptor is located (Fig. 4c). Moreover, the cleft between the two domains would remain accessible, consistent with the biochemical requirement that the soluble UDP-GlcNAc donor be able to find its binding site from the cytoplasm.

Implications for other glycosyltransferases

Glycosyltransferases that utilize an activated nucleotide sugar as a donor comprise a large family of enzymes in both prokaryotes and eukaryotes, and they play central roles in many important biological processes (Dennis *et al.*, 1999; Koya *et al.*, 1999; Verbert & Cacan, 1999). Glycosyltransferases are typically classified according to the nucleotide sugar they utilize, and it has frequently been noted that there is no significant sequence homology even among glycosyltransferases in the same family. This has made it difficult to identify common structural features and residues important in binding and catalysis. There are only three other glycosyltransferase structures available, and although none of them shows any sequence homology to MurG, a structural comparison indicates that one of them, BGT, contains a related donor binding site.

In addition to this structural homology, we have identified a strikingly similar sequence motif in the MurG family and certain other UDP-glycosyltransferase families. This sequence motif spans about a thirty amino acid stretch in the C-domain of MurG and includes most of the invariant residues found in that domain. As shown in Figure 3a, a similar motif is found in the UDP-glucuronosyltransferases (Mackenzie, 1990). Certain residues are identical, including a number of prolines and glycines, and the spacing between them is invariant. This suggests that the UDP-glucuronosyltransferases contain a region of ?/? supersecondary structure that is involved in a similar function as the corresponding region in MurG (Fig. 3c). This region binds the donor sugar. By analyzing the similarities and differences between the conserved residues in this subdomain in the MurG family and other UDP-glycosyltransferase families, it may be

possible to identify – and perhaps alter - residues that are involved in determining donor selectivity. We note that it would be useful to be able to manipulate donor specificity because it would extend the utility of glycosyltransferases as reagents for glycosylation of complex molecules. Altered glycosyltransferases could also be useful for remodeling cell surfaces and for probing the biological roles of particular carbohydrate structures.

Conclusion

This first structure of a member of the MurG family of glycosyltransferases lays the groundwork for further mechanistic and structural investigations, which may lead to the design of inhibitors and perhaps even new antibiotics. The work also shows that there can be conserved subdomains even in very different glycosyltransferase families. Information on conserved subdomains will be useful for structure prediction and may help guide experiments directed towards changing substrate specificity.

EXAMPLE 2

This example describes a method of isolating the C-terminal domain of the *E. coli* MurG protein, expressing the domain in *E. coli* cells and utilizing nuclear magnetic resonance (NMR) to determine the ability of compounds to bind.

MurG can also be used to determine the ability of a chemical compound to bind to the C domain by a) determining the start of c domain based on the MurG crystal structure; b) independently expressing the C domain; and c) using NMR methods to identify binding site and/or bound conformation of ligand. The same procedure is used for the acceptor binding domains.

NMR methods are used to identify the protein binding sites nad screen for ligands that bind. The MurG C-terminal domain region of the protein has been expressed independently. The C domain has a much lower molecular weight than the full-length protein. Therefore, the expression of the C domain results in much sharper NMR peaks which will facilitate the NMR interpretation. Also the protin chemical shifts are very sensitive to their environment. Binding of a compound will introduce local environment changes, thus changing the proton chemical shifts. In this way, residues involved in the binding can be differentiated easily from other amino acid residues not involved in

binding a ligand. This method has also been used to identify ligands that bind to low molecular weight drug targets (i.e., small proteins).

Relevant references to NMR techniques are: Discovering high-affinity ligands for proteins: SAR by NMR, S. Shuker, P. Hajduk, R. Meadows, and S. Fesik, Science 274, 1531 (1996); Lin Y, Nageswara Rao BD. Structural characterization of adenine nucleotides bound to Escherichia coli adenylate kinase. 1. Adenosineconformations by proton two-dimensional transferred nuclear Overhauser effect spectroscopy. Biochemistry. 2000 Apr 4;39(13):3636-46; and Fejzo J, et al., Chem Biol 1999 Oct;6(10):755-69 (incorporated herein by reference).

The SHAPES strategy is also useful for NMR identification of binding residues, ligands and drug discover which is an NMR-based approach for lead generation in drug discovery. Recently, it has been shown that nuclear magnetic resonance (NMR) may be used to identify ligands that bind to low molecular weight protein drugtargets. Recognizing the utility of NMR as a very sensitive method for detecting binding, we have focused on developing alternative approaches that are applicable to larger molecular weight drug targets and do not require isotopic labeling. A new method for lead generation (SHAPES) uses NMR to detect the binding of a limited but diverse library of small molecules to a potential drug target. The compound scaffolds are derived from shapes most commonly found in known therapeutic agents. NMR detection of low (microM-mM) affinity binding is achieved using either differential line broadening or transferred NOE (nuclear Overhauser effect) NMR techniques. The SHAPES method for lead generation by NMR is useful for identifying potential lead classes of drugs early in a drug design program, and is easily integrated with other discovery tools such as virtual screening, high-throughput screening and combinatorial chemistry.

EXAMPLE 3

This example describes the method of using the three-dimensional structure of *E. coli* MurG to determine the crystal structures of its mutant, enzyme-ligand complex, and MurG homologs, which share the same folding motif.

First, a crystalline form of the new protein or the protein complex should be obtained. The E.coli MurG mutants should crystallized in a condition very similar to

what we have showed in the method section. The protein-ligand complex can be obtained by soaking the protein crystals in a ligand-containing buffer. Other MurG homologs can be expressed in a His-tagged fashion and purified using affinity colume. Presumably they can be crystallized in a similar way using a detergent as the additive. Next, the diffraction data should be collected and processed. After the data collection, the molecular replacement method is used to determine the unknown structure. Either the whole E. coli MurG protein or one single domain can serve as a search model. This search model can be rotated and translated until the correct orientation is located in the unit cell of this unknown structure. The search model may only represent part of the contents of the asymmetric unit. However, the location of the first model is now already available. While the first location of the search model is fixed, the second round of translation search can be carried out to search more molecules or domains in the asymmetric unit cell. The phases from the final model generated by molecular replacement can be used to calculate the electron density map. Finally, a model is built based on the electron density map, and the model needs to be refined using program CNS or XPLOR.

EXAMPLE 4

This example describes the method of using the three-dimensional coordinate structure of E. coli MurG to produce a protein fragment that can be used in an NMR-based lead discovery program. The crystal structure reveals the boundaries of the C domain and permits us to design a gene containing only the C domain from the gene containing both domains. The C domain starting at residue 164 and ending at residue 340 was cloned into an expression vector to generate a C-terminal His tag fusion. It was over-expressed in E. coli cells and purified by affinity colume. The protein was shown to be monomeric by size exclusion chromatography and to be soluble at least up to 0.15 mM, a concentration more than adequate for NMR analysis. C domains from other Murg homologues can be similarly expressed and used.

EXAMPLE 5

This example describes the co-crystallization of a MurG protein with a ligand. A MurG-ligand complex is formed by either co-crystallizing MurG protein with appropriate ligand or soaking the MurG crystals in buffers containing appropriate ligand. Co-crystallization is done by pre-mixing the protein sample with a certain amount of substrate or substrate analogs. Then the hanging drop method is used to produce crystals as described infra.

Alternatively, ligans are incorporated into the crystals by soaking the protein crystals in the ligand containing buffer for a period of time to allow for infiltration into the crystal. The time ranges from a couple of hours to a couple of days. The concentration of ligand in the buffer ranges from several milimolar to several hundred mili molar.

DEPOSIT OF COORDINATES

The crystal structure three-dimensional coordinates of the *E. coli* MurG as set forth in Table 1 were deposited with the Protein Data Bank and have been assigned the indicated ID Code (Accession No.) 1F0K.

Although the invention is described in detail with reference to specific embodiments thereof, it will be understood that variations which are functionally equivalent are within the scope of this invention. Indeed, various modifications of the invention in addition to those shown and described herein will become apparent to those skilled in the art from the foregoing description and accompanying drawings. Such modifications are intended to fall within the scope of the appended claims.

Various publications are cited herein, the disclosures of which are incorporated by reference in their entireties.

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WHAT IS CLAIMED IS:

1. A composition comprising the *E. coli* MurG protein in crystalline form.

2. A composition comprising a MurG protein in crystalline form.

3. A three dimensional structure of the crystalline form of an *E. coli* MurG protein, wherein the three dimensional structure substantially conforms to the atomic coordinates represented in Table 1.

4. A three dimensional structure of the crystalline form of a MurG protein, wherein the three dimensional structure substantially conforms to the atomic coordinates represented in Table 1.

5. A three dimensional structure of the α-carbon backbone of the crystalline form of an *E. coli* MurG protein, wherein the three dimensional structure substantially conforms to the atomic coordinates represented in Table 2.

6. A three dimensional structure of the α-carbon backbone and conserved amino acid residues of an *E .coli* MurG protein, wherein the three dimensional structure substantially conforms to the atomic coordinates represented in Table 3.

7. A three dimensional structure of a donor nucleotide binding site of a MurG protein wherein the three dimensional structure structure of the donor nucleotide binding site substantially conforms to the atomic coordinates in Table 4.

8. The three dimensional structure of claim 7, wherein the donor nucleotide is UDP-GlcNAc.

9. A three dimensional structure of an acceptor binding site of a MurG protein substantially conforming to the atomic coordinates in Table 5.

10. A three dimensional structure of a membrane association site of a MurG protein substantially conforming to the atomic coordinates in Table 6.

11. A three-dimensional computer image of the three-dimensional structure of a MurG protein.

12. The image of claim 11, wherein the structure substantially conforms with the three-dimensional coordinates listed in Table 1.

13. The image of claim 11, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software

program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

14. The image of claim 11, wherein the three-dimensional computer image is represented by a two dimensional image selected from the group consisting of Fig. 2a, 3a, or 4c.

15. The image of claim 11, wherein the three-dimensional computer image is used to design a compound.

16. A three dimensional computer image of the three dimensional structure of the α-carbon backbone of a MurG protein.

17. The image of claim 16, wherein the structure substantially conforms with the three-dimensional coordinates listed in Table 2.

18. The image of claim 16, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 2 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

19. The image of claim 16, wherein the three-dimensional computer image is used to design a compound.

20. A three dimensional image of the three dimensional image of an α-carbon backbone and conserved amino acid residues of a MurG protein.

21. The image of claim 20, wherein the structure substantially conforms with the three-dimensional coordinates in Table 3.

22. The image of claim 21, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 3 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

23. The image of claim 21, wherein the three-dimensional computer image is used to design a compound.

24. A three-dimensional computer image of the three-dimensional structure of a donor nucleotide binding site of a MurG protein.

25. The image of claim 24, wherein the structure substantially conforms with the three-dimensional coordinates in Table 4.

26. The image of claim 24, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 4 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

27. The image of claim 24, wherein the three-dimensional computer image is represented by a two dimensional image selected from the group consisting of Fig. 3c, 4a or 4b.

28. The image of claim 24, wherein the three-dimensional computer image is used to design a compound.

29. A three-dimensional computer image of the three-dimensional structure of an acceptor binding site of a MurG protein.

30. The image of claim 29, wherein the structure substantially conforms with the three-dimensional coordinates Table 5.

31. The image of claim 29, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 5 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

32. The image of claim 29, wherein the three-dimensional computer image is represented by the two dimensional image of Fig. 4a.

33. The image of claim 29, wherein the three-dimensional computer image is used to design a compound.

34. A three-dimensional computer image of the three-dimensional structure of a membrane association site of a MurG protein.

35. The image of claim 34, wherein the structure substantially conforms with the three-dimensional coordinates Table 6.

36. The image of claim 34, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 6 are analyzed on a computer using a graphical display software

program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

37. The image of claim 34, wherein the three-dimensional computer image is represented by the two dimensional image of Fig. 4a.

38. The image of claim 34, wherein the three-dimensional computer image is used to design a compound.

39. A computer readable medium encoded with a set of three-dimensional coordinates of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 1, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

40. A computer readable medium encoded with a set of three-dimensional coordinates of an α-carbon backbone of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 2, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

41. A computer readable medium encoded with a set of three-dimensional coordinates of an α-carbon backbone and conserved amino acid residues of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 3, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

42. A computer readable medium encoded with a set of three-dimensional coordinates of a donor nucleotide binding site of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 4, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

43. A computer readable medium encoded with a set of three-dimensional coordinates of an acceptor binding site of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5, wherein using

a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image..

44. A computer readable medium encoded with a set of three-dimensional coordinates of a membrane association site of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image.

45. A method for identifying a potential inhibitor of a UDP-glycosyltransferase enzyme, the method comprising the steps of:

a. using a three-dimensional structure of UDP-glycosyltransferase enzyme as defined by atomic coordinates of UDP-glycosyltransferase enzyme according to FIG. 5;

b. employing said three-dimensional structure to design or select said potential inhibitor;

c. synthesizing said potential inhibitor; and

d. contacting said potential inhibitor with said UDP-glycosyltransferase enzyme in the presence of a substrate to test the ability of said potential inhibitor to inhibit said UDP-glycosyltransferase enzyme.

46. The method according to claim 45, wherein said potential inhibitor is selected from a database.

47. The method according to claim 45, wherein said potential inhibitor is designed de novo.

48. The method according to claim 45, wherein said potential inhibitor is designed from a known inhibitor.

49. The method according to claim 45, wherein said step of employing said three-dimensional structure to design or select said potential inhibitor comprises the steps of:

a. identifying chemical entities or fragments capable of associating with UDP-glycosyltransferase enzyme; and

b. assembling the identified chemical entities or fragments into a single molecule to provide the structure of said potential inhibitor.

50. The method according to claim 45, wherein the potential inhibitor is a competitive inhibitor of mutant UDP-glycosyltransferase enzyme.

51. The method according to claim 45, wherein said potential inhibitor is a non-competitive or uncompetitive inhibitor of mutant UDP-glycosyltransferase enzyme.

52. A model of a UDP-glycosyltransferase, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 1.

53. The model of claim 52, wherein the structure substantially conforms to the atomic coordinates and B-values represented by Table 1.

54. The model of claim 52, wherein the structure is monomeric.

55. The model of claim 52, wherein at least about 50% of the structure has an average root-mean-square deviation (RMDS) of less than about 2.5 Å for backbone atoms in secondary structure elements in each domain of the structure.

56. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 25% identical to the amino acid sequence of the *E. coli* MurG protein.

57. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 40% identical to the amino acid sequence of the *E. coli* MurG protein.

58. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 60% identical to the amino acid sequence of the *E. coli* MurG protein.

59. The model of claim 52, wherein the MurG protein comprises an amino acid sequence selected from the group consisting of the amino acid sequence of a MurG protein from *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime*, and *Treponema pallidum*, a mutant of any of the amino acid sequences, and a variants of any of the amino acid sequences.

60. The model of claim 52, wherein the MurG protein comprises an amino acid sequence selected from the group consisting of the amino acid sequences of MurG proteins as deposited in the NCBI database and identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552,)67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436.

61. The model of claim 52, wherein the MurG protein comprises an amino acid sequence obtained from an organism selected from the group consisting of bacteria, small pathogenic organisms, cyano bacteria, higher-order bacteria, spirochetes and thermal stable bacteria.

62. The model of claim 52, wherein the MurG protein comprises an amino acid sequence obtained from an organism selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

63. The model of claim 52, wherein the MurG protein is a structural homologue of the *E. coli* MurG protein.

64. The model of claim 52, wherein the structure comprises an n-terminal and C-terminal domain connected by a covalent peptide linker, and wherein each domain has an alpha/beta fold.

65. The model of claim 52, wherein the RMSD is less than 2.5 Å over at least 80 aligned C-alpha atoms in each domain.

66. The model of claim 52, wherein the N-terminal domain comprises two glycine rich loops.

67. The model of claim 66, wherein the amino acid sequence of the two glycine rich loops comprises GGTGGH and G-GGYVSG.

68. The model of claim 52, wherein the C-terminal domain comprises one glycine rich loop.

69. The model of claim 68, wherein the glycine rich loop comprises the amino acid sequence GGSQGAR or GGS-GAR.

70. The model of claim 52, wherein the atomic coordinates are generated by the method comprising the steps of:

(a) providing a MurG protein in crystalline form;

(b) generating an electron-density map of the crystalline MurG protein; and

(c) analyzing the electron-density map to produce the atomic coordinates.

71. The model of claim 70, wherein the crystalline MurG protein is produced by a method comprising the steps of:

(a) combining MurG protein with UDP-GlcNAc ,and

(b) inducing crystal formation to produce said crystalline MurG protein.

72. The model of claim 70, wherein the crystalline MurG protein is produced by the hanging drop method in which MurG in buffer is at a concentration of at least 5 ug/ml and is combined with a reservoir solution and crystallizes.

73. The model of claim 72, wherein the buffer has a pH range from about 6.5 to about 9.0, and a buffer concentration range from about 10 mM to about 200 mM.

74. The model of 73, wherein the buffer is a Tris or a Hepes buffer, having a pH from about 7.0 to about 8.5.

75. The model of 74, wherein the buffer has a pH of about 7.9.

76. The model of claim 73, wherein the buffer further comprises at least one salt, chelating agent, or reducing agent.

77. The model of claim 72, wherein the reservoir solution has a pH range from about 5.0 to about 9.0 and the buffer concentration ranges from about 10 mM to about 1M.

78. The model of claim 77, wherein the reservoir solution further comprises at least one suitable precipitant, a detergent, and a reducing agent.

79. The model of claim 78, wherein the reservoir solution comprises a NaMES or sodium citrate buffer having a pH from about 6.0 to about 7.0.

80. The model of claim 79, wherein the buffer has a pH of about 6.5.

81. The model of claim 78, wherein the precipitant is selected from the group consisting of ammonium sulfate and sodium potassium tartrate.

82. The model of 78, wherein the detergent is TritonX-100.

83. The model of 78, wherein the reducing agent is DTT, DTE or beta-mercaptoethanol.

84. The model of claim 71, wherein the MurG protein and the UDP-GlcNAc are in a 1:3 molar ratio.

85. The model of claim 71, wherein the buffer comprises 0.1 M NaMES, pH6.5, 0.9M $(NH_4)_2SO_4$, 0.4% TRITON X-100®, and 10 mM dithiothreitol (DTT).

86. The model of claim 71, wherein the step of generating an electron-density map comprises analyzing the crystalline MurG protein by X-ray diffraction.

87. The model of claim 70, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

88. A model of a donor nucleotide binding site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 4.

89. The model of claim 88, wherein the donor nucleotide binding site is located within the MurG C-terminal domain.

90. The model of claim 88, wherein the structure substantially conforms to the atomic coordinates and B-values of Table 4.

91. The model of claim 88, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 2.5Å for the conserved amino acid residues for the donor nucleotide binding site of the E. coli MurG.

92. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the donor nucleotide binding site of E. coli MurG.

93. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the donor nucleotide binding site of the E. coli MurG.

94. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the donor nucleotide binding site of the E. coli MurG.

95. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of the donor nucleotide binding site of the E. coli MurG.

96. The model of claim 88, wherein the atomic coordinates are generated by a method comprising the steps of:

a) providing a Murg protein in a crystalline form:

b) generating an electron-density map of said crystalline MurG protein; and

c) analyzing the electron-density map to produce the atomic coordinates.

97. The model of claim 88, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

98. A model of an acceptor binding site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5 .

99. The model of claim 98, wherein the structure substantially conforms to the atomic coordinates and B-values of Table 5.

100. The model of claim 98, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 1.5Å for the conserved amino acid residues in the acceptor binding site.

101. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the acceptor binding site of E. coli MurG.

102. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the acceptor binding site of E. coli MurG.

103. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the E. coli MurG.

104. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of the acceptor binding site of the E. coli MurG.

105. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 70% identical to the amino acid sequence selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime*, and *Treponema pallidum*.

106. The model of claim 98, wherein the atomic coordinates are generated by the method comprising the steps of:

a) providing a MurG protein in a crystalline form:

b) generating an electron-density map of said crystalline MurG protein; and

c) analyzing the electron-density map to produce the atomic coordinates.

107. The model of claim 98, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

108. A model of a membrane association site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 6.

109. The model of claim 108, wherein the structure substantially conforms to the atomic coordinates and B-values of Table 4.

110. The model of claim 108, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 1.5Å for conserved amino acid residues in the E. coli membrane association site.

111. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the membrane association site of E. coli MurG.

112. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the membrane association site of the E. coli MurG.

113. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the membrane association site of the E. coli MurG.

114. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of a membrane association site of the E. coli MurG.

115. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 70% identical to the amino acid sequence from organisms selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

116. The model of claim 108, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

117. A computer-assisted method of structure based drug design of bioactive compounds, comprising the steps of:

(a) providing a model of a UDP-glycosyltransferase (MurG)protein or a donor nucleotide binding site, acceptor binding site or membrane association site; and

(b) designing a chemical compound using said model.

118. The method of claim 117, further comprising the step of synthesizing the chemical compound.

119. The method of claim 118, further comprising the step of evaluating the bioactivity of the synthesized chemical compound.

120. The method of claim 118, wherein the model of the UDP-glycosyltransferase (MurG) protein represents a three-dimensional structure comprising the atomic coordinates listed in Table 1.

121. The method of claim 118, wherein the model of the donor nucleotide binding site represents a three-dimensional structure comprising the atomic coordinates Table 4.

122. The method of claim 118, wherein the model of the acceptor binding site represents a three-dimensional structure comprising the atomic coordinates in Table 5.

123. The method of claim 118, wherein the model of the membrane association site represent a three-dimensional structure comprising the atomic coordinates in Table 6.

124. The method of claim 118, wherein the model comprises a computer image generated when the atomic coordinates listed in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

125. The method of claim 118, wherein the step of designing comprises computational screening of one or more databases of chemical compounds in which the three dimensional structure of said compounds are known.

126. The method of claim 125, further comprising interacting a compound identified by the screening step with the model by computer.

127. The method of claim 118, wherein the step of designing comprises directed drug design.

128. The method of claim 118, wherein the step of designing comprises random drug design.

129. The method of claim 118, wherein the step of designing comprises grid-based drug design.

130. The method of claim 118, wherein the step of designing comprises selecting compounds which are predicted to mimic the three-dimensional structure of the three-dimensional structure of the MurG protein.

131. The method of claim 118, wherein the step of designing comprises selecting compounds which are predicted to bind to the three-dimensional structure of the MurG protein.

132. The method of claim 118, wherein the bioactivity is selected from the group consisting of inhibiting binding of a nucleotide donor compound to the MurG protein,

inhibiting binding of an acceptor compound to the MurG protein, or inhibiting association of the MurG Protein to a membrane.

133. A model of the three dimensional structure of a MurG protein , wherein the model is produced by the following method comprising the steps of:

(a) providing an amino acid sequence of a MurG protein and the amino acid sequence of the *Escherichia coli* MurG protein;

(b) identifying structurally conserved regions shared between the the MurG protein and the E. coli MurG protein; and

(c) determining atomic coordinates for the MurG protein by assigning the structurally conserved regions of the MurG protein to a three dimensional structure using a three dimensional structure of the MurG protein which substantially conforms to the atomic coordinates represented in Table 1, to derive a model of the three dimensional structure of the MurG protein amino acid sequence.

134. The model of claim 133, wherein the MurG protein amino acid sequence comprises the sequence of an amino acid sequence selected from the group consisting of the amino acid sequences of MurG proteins as deposited in the NCBI database and identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552,)67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436.

135. A composition for inhibiting the activity of a glycosyltransferase comprising a compound that inhibits the activity of a glycosyltransferase, wherein the compound is identified by the method comprising the steps of:

(a) providing a three-dimensional structure of a MurG protein;

(b) using the three-dimensional structure of the MurG protein to design a chemical compound that inhibits activity of a glycosyltransferase;

(c) synthesizing the chemical compound; and

(d) evaluating the ability of the chemical compound to inhibit the activity of a glycosyltransferase.

136. e composition of claim 135, wherein the glycosyltransferase is a MurG protein.

137. The composition of claim 135, wherein the three-dimensional structure of the MurG protein substantially conforms to atomic coordinates represented by Table 1.

138. The composition of claim 135, wherein the compound is selected from the group consisting of an inorganic and an organic compound.

139. The composition of claim 135, wherein the compound is a substituted pyrimidine analogs

140. The composition of claim 135, wherein the compound is selected from the group consisting of an analog of a MurG protein, a substrate analog of a MurG protein, a donor molecule analog of a MurG protein, and a membrane analog of a MurG protein.

141. The composition of claim 135, further comprising a component selected from the group consisting of an excipient an adjuvant, and a carrier.

142. A composition for stimulating the activity of a glycosyltransferase comprising a compound that stimulates the activity of a glycosyltransferase, wherein the compound is identified by the method comprising the steps of:

(a) providing a three-dimensional structure of a MurG protein;

(b) using the three-dimensional structure of the MurG protein to design a chemical compound that inhibits activity of a glycosyltransferase;

(c) synthesizing the chemical compound; and

(d) evaluating the ability of the chemical compound to stimulate the activity of a glycosyltransferase.

143. A method to determine a three-dimensional structure of a MurG protein comprising the steps of:

(a) providing an amino acid sequence of a MurG protein, wherein the three-dimensional structure of the MurG protein is not known;

(b) analyzing the pattern of folding of the amino acid sequence in a three-dimensional conformation by fold recognition; and

(c) comparing the pattern of folding of the MurG protein amino acid sequence with the three dimensional structure of the E. coli MurG protein, wherein the three-dimensional structure of the E. coli MurG protein substantially conforms to the atomic coordinates represented in Table 1.

144. A method to derive a model of the three-dimensional structure of a MurG protein comprising the steps of:

(a) providing an amino acid sequence of a MurG protein;

(b) identifying structurally conserved regions shared between the MurG protein and the E. coli MurG protein;

(c) determining atomic coordinates for the MurG protein structure by assigning the structurally conserved regions of the MurG protein to a three-dimensional structure using a three dimensional structure of the E. coli MurG protein based on atomic coordinates represented in Table 1 to derive a model of the three dimensional structure of the MurG protein amino acid sequence.

145. The method of claim 144, further comprising assigning atomic coordinates for side chains of said MurG protein by determining sterically allowable positions using a library of rotamers.

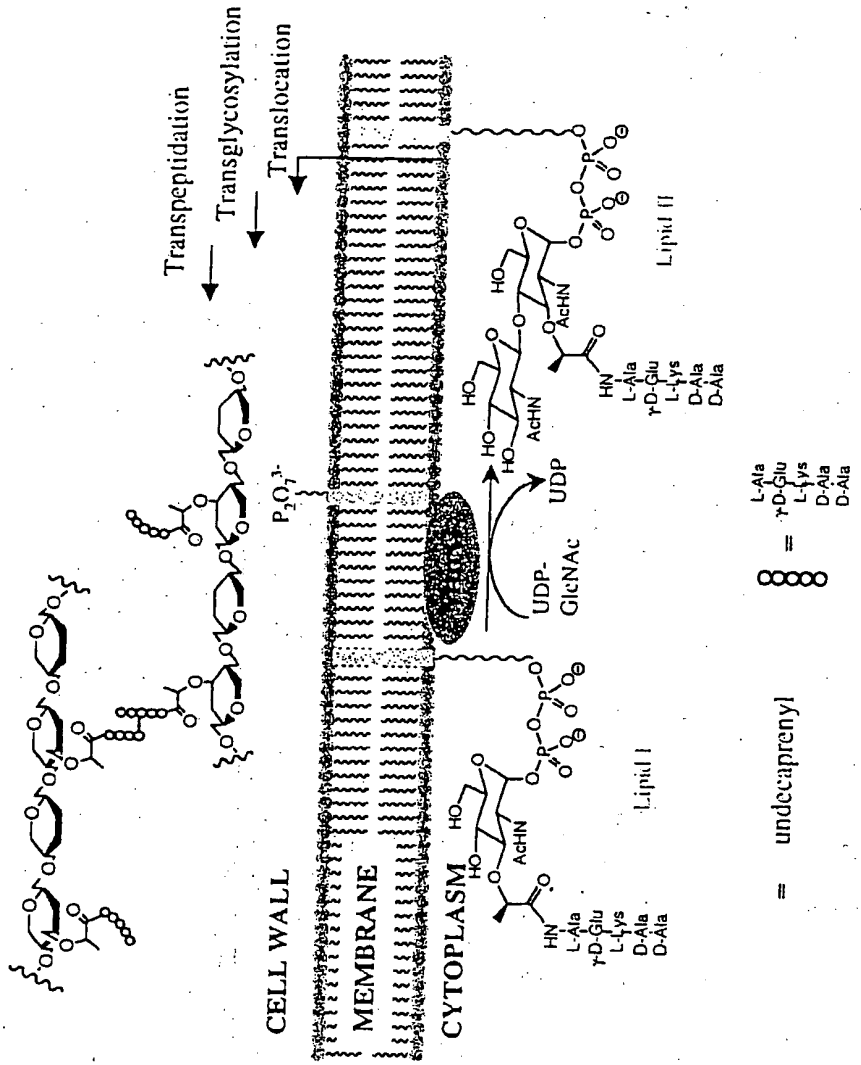
146. A method to derive a three dimensional structure of a crystallized MurG protein comprising the steps of:

(a) comparing the Patterson function of a crystallized MurG protein with the Patterson function of crystalline E. coli MurG protein to produce an electron-density map of the crystallized MurG protein; and

(b) analyzing the electron-density map to produce the three dimensional structure of the crystallized MurG protein.

147. The method of claim 146, further comprising the step of rotating the Pattersor function of the crystallized MurG protein on the Patterson function of the crystalline E coli MurG protein to determine the correct orientation of the crystallized MurG proteir in a crystal of said crystallized MurG protein to identify the initial phases of the crystallized MurG protein.

148. The method of claim 146, further comprising the step of electronically stimulating the three dimensional structure of the crystallized MurG protein to derive a computer image of the three dimensional structure of the crystallized MurG protein.


Transpeptidation
Transglycosylation
Translocation
CELL WALL
MEMBRANE
CYTOPLASM
$P_2O_7^{3-}$
UDP-GlcNAc
UDP
Lipid I
Lipid II
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γ-D-Glu
L-Lys
D-Ala
D-Ala
AcHN
HO
= undecaprenyl

Fig. 1

Fig. 2a

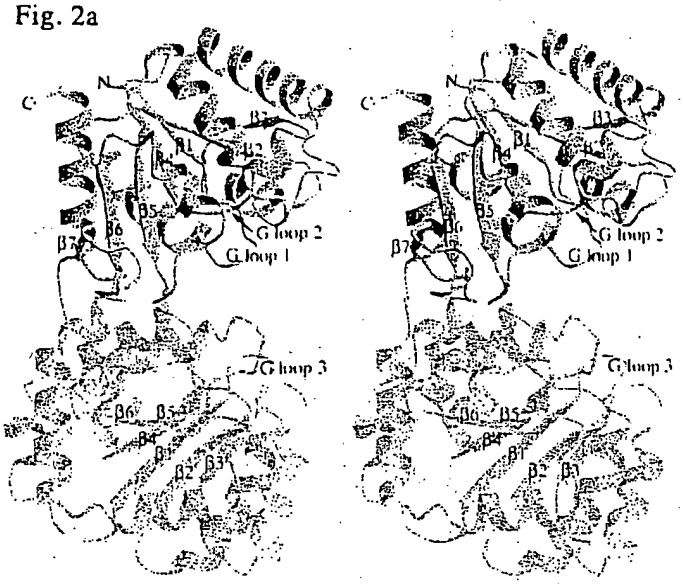
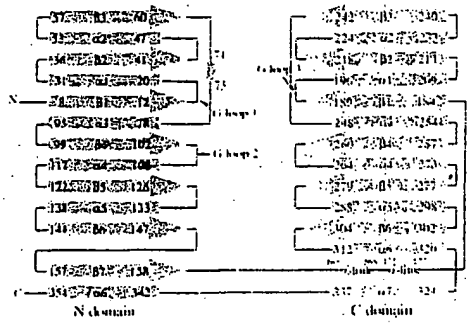


Fig. 2b



E. coli
Haemophilus influenzae
Enterococcus faecalis
Enterococcus hirae
Streptococcus pneumoniae
Rickettsia prowazekii
Bacillus subtilis
Mycobacterium tuberculosis
Consensus
UDP-Glucuronosyltransferase consensus region

Fig. 3a

Fig. 3b

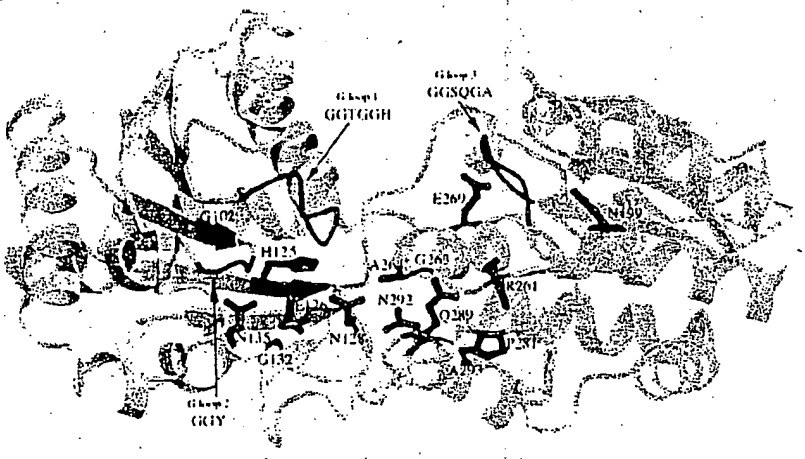
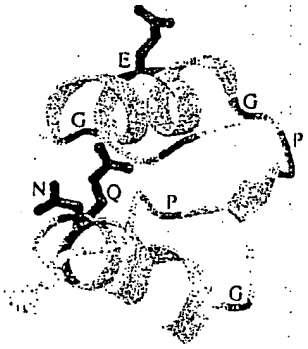
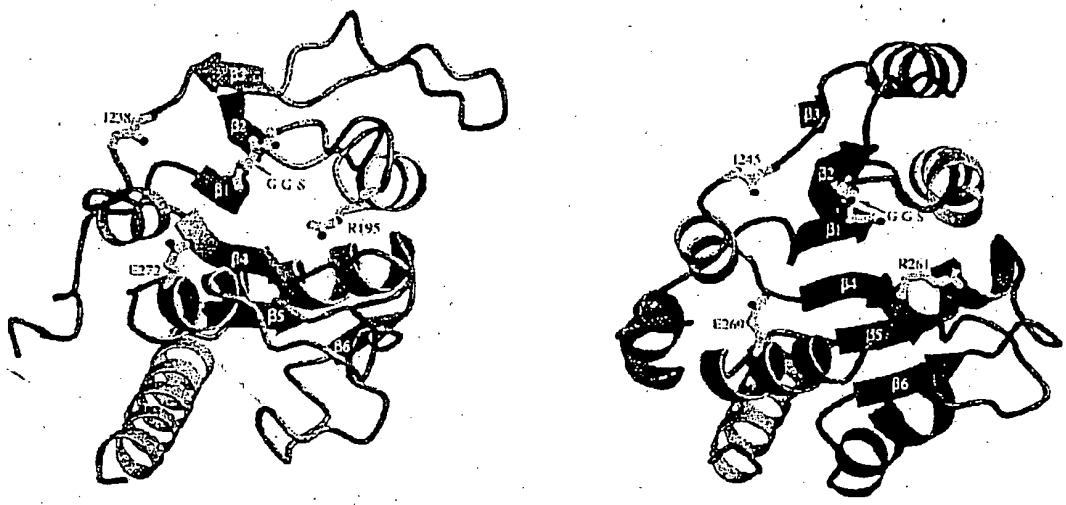


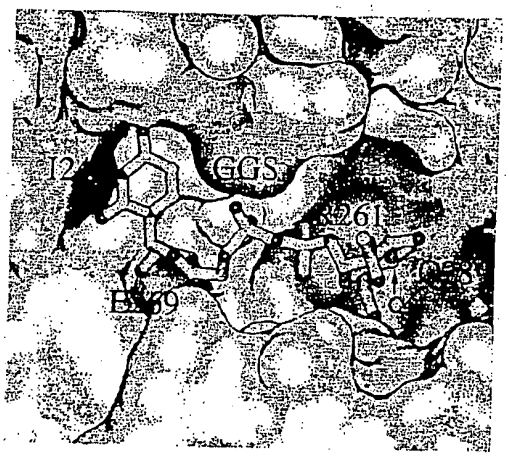
Fig. 3c



A


GGS
R195
GGS
R261

B


GGS

C

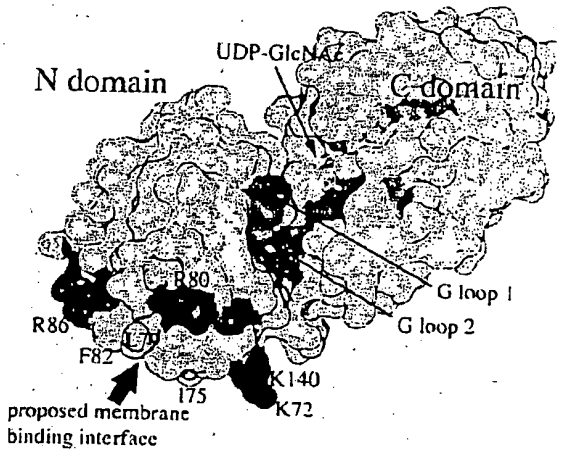

UDP-GlcNAz
N domain
C domain
R80
G loop 1
G loop 2
R86
F82
K140
175
K72
proposed membrane
binding interface

Fig. 4